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Sachplan Geologische Tiefenlager, Etappe 3

Recommendations for Supplementary Investigations related to Repository Gas Transport in the Opalinus Clay

September 11th, 2020

Expertengruppe Geologische Tiefenlagerung (EGT)

Sachplan Geologische Tiefenlager, Etappe 3

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Table of Contents

1. Introduction 3

1.1 Study Framework and Objectives 3

1.2 Study Authors 4

2. Observations of Hydrocarbon Gas Leaks and Induced Seismicity of Fault Zones cross-cutting Clay Shales 5

2.1 Global Observations 5

2.2 The St. Gallen Geothermal Well 5

3. Structure and Fabric of Steep Fault zones in the Proposed Siting Regions 9

4. Strength, Dilatancy and Criticality of Fault Rocks in the Opalinus Clay 12

4.1 Strength and Dilatancy of Mont Terri Rock Samples 12

4.2 Fault Slip at Mont Terri 13

4.3 Criticality of Opalinus Clay Faults in the Alpine Foreland 14

5. Gas production in the HLW and L/ILW Repositories 16

5.1 Gas Production in the HLW Repository 16

5.2 Gas Production in the L/ILW Repository 16

5.3 EGT Evaluation 18

6. Gas Transport and Pore Pressure Build-up in the Opalinus Clay 19

6.1 Gas Transport and Pore Pressure Simulations 19

6.2 Model Input Parameters 22

6.3 Recommended Supplementary Investigations 23

7. Gas related Post-Closure Safety Functions and Evaluation Criteria 25

7.1 Porewater Displacement 25

7.2 Pathway Dilation 25

7.3 Gas Fracking 26

7.4 Gas Leakage and Shearing of Critically Stressed Faults 26

8. Summary of Recommendations 28

8.1 Preamble 28

8.2 Detailed recommendations of EGT 28

9. References 31

Figure 1: Summary figure with seismicity St Gallen geothermal well 7

1. Introduction

1.1 Study Framework and Objectives

EGT (Expertengruppe Geologische Tiefenlagerung) is the Swiss scientific-technical expert group for nuclear waste disposal, supporting the Swiss Regulator ENSI (Eidgenössisches Nuklearsicherheitsinspektorat) in reviewing the projects and license applications of the nuclear waste disposal implementer Nagra, in regulation and review procedures, and in the supervision of field activities. EGT is composed of 7-10 international experts, mainly from research institutions, and is independent from the implementer Nagra.

The annual working program is developed together with ENSI and based on at least 5 closed full-day plenary meetings. The results of the work carried out by EGT are published as open-file reports, short statements and contributions to hearings and scientific conferences.

A major topic of EGT in 2019 and 2020 was an in-depth analysis of repository gas related issues, mainly in the context of Stage 3 of the Sectoral Plan for Geological Repository Site Selection (SGT, Sachplan Geologische Tiefenlager, BFE 2011). Stage 3 of this plan deals with the final selection of the best location for a HLW and I/LLW repository in Northern Switzerland. Field investigations related to site selection are supposed to be completed in 2021; and the selected final repository sites are expected to be proposed by Nagra in 2022.

Although all possible locations evaluated in Stage 3 are in the same host rock (Opalinus Clay), repository-related gas issues might differ between the proposed sites. Stage 3 is the last stage that involves substantial field investigations before the general license application (Rahmenbewilligungsgesuch), when an in-depth safety analysis has to be provided by the implementer. This safety analysis has to demonstrate long term safety of both repository types including all possible negative effects of repository gas generation. Therefore, the field and subsequent lab investigations of Stage 3 also have to provide all necessary data for the analysis of gas related safety functions, such as gas pressure build-up, gas transport and brine displacement.

The goal of this report is to critically evaluate if additional field and laboratory data have to be collected during Stage 3 of the SGT, which are needed for the site selection in 2022 and the general license application due in 2024. This evaluation is not only based on the safety indicator criteria applied in Stage 1 and 2 of the SGT (NTB 08-05), but on a broader review of gas-related transport observations along steeply dipping fault zones in clay rock. It represents an extension of the EGT Stage 2 review report (EGT 2017) and contains a detailed analysis of gas transport mechanisms and relevant tectonic structures in the Opalinus Clay. Not discussed in this report are technical issues, such as the Engineering Gas Transport System, proposed by Nagra (NAB 14-16). This system will be studied and evaluated by EGT in 2021.

A major topic of this report is gas transport through clay caprocks and steeply dipping faults. This topic is first introduced in Chapter 2, based on a review of selected global and Swiss observations. Chapter 3 discusses the current knowledge about critical properties of steep fault zones in the proposed siting regions, and Chapter 4 evaluates the available rock mechanical and hydromechanically coupled data from Opalinus Clay fault rocks. In Chapter 5 the expected gas production rates for the HLW and L/ILW repository are reviewed, which leads to a critical discussion of modeled gas pressure build-up, and gas/brine transport in the Swiss disposal concept (Chapter 6). The relevance of the different gas related scenarios and indicators for long term repository safety is discussed in Chapter 7, leading to a summary of EGT recommendations for supplementary field and lab investigations in Stage 3 of the SGT (Chapter 8).

1.2 Study Authors

This report has been written by the following EGT experts:

Prof. Dr. Simon Löw: Chapters 1, 2, 4, 7, 8

Prof. em. Dr. Neil Mancktelow: Chapters 2, 3, 4, 8

Prof. Dr. Horst Geckeis: Chapters 5, 8

Prof. Dr. Rainer Helmig: Chapters 6, 8

Prof. em. Dr. Friedemann Wenzel: Chapters 3, 8

The appendix has been provided by an external expert for multi-phase flow in clay shales (Prof. Dr. Russel Johns). The entire report has been reviewed by all members of EGT. This project was led by the EGT Chairman Simon Löw.

2. Observations of Hydrocarbon Gas Leaks and Induced Seismicity of Fault Zones cross-cutting Clay Shales

2.1 Global Observations

The Opalinus Clay is the selected host rock for nuclear waste repositories in Switzerland with expected sealing functions similar to those of a shale caprock in a liquid or gaseous hydrocarbon reservoir. Accumulated experience from the petroleum industry on the self-sealing properties of faults and fractures within argillaceous (shaly) caprocks can therefore provide a good basis for considering the behaviour of gas in the Opalinus Clay at depth within the potential siting areas (e.g. NAB 13-06). Evans (2007) discusses two types of failure mechanisms of such caprocks: membrane seal failure corresponding to gas transport through the pre-existing pore structure of the caprock (either by solution in groundwater or as two-phase flow), and hydraulic seal failure corresponding to hydraulic failure of the caprock, eventually associated with fault reactivation. Leak-off tests in wells have shown that gas opens existing fractures when gas pressure gradients are between 22.6 and 24.9 kPa/m (Evans 2007), which is close to lithostatic pressure for a sedimentary reservoir environment. As summarized in NAB 13-06, page 3), the top seals to petroleum reservoirs that are "fill to spill" and clay-rich sediments around potential radioactive waste disposal sites appear to have lower overconsolidation ratios (OCR, 1-2.5) than the shale gas reservoirs (2-5.5). However, there is evidence that shallowly buried top seals that have not been embrittled by late stage diagenetic processes (i.e. diagenetic processes that occur during deep burial) can remain good seals despite having OCR's >2.5. With specific reference to the Opalinus Clay, NAB 13-06 notes on page 55 that "based on OCR, the Opalinus Clay in Benken (OCR~1.5-2.5) would be thought of as being borderline regarding its susceptibility to deforming to create fault and fracture-related conduits. On the other hand, the Opalinus Clay in Mont Terri would be viewed as high risk of leakage as its OCR is 2.5-3.5. However, there is also evidence that top seals that have not been embrittled by deep burial can remain good seals despite deforming when severely overconsolidated". At long time scales (millions of years), all caprocks are supposed to leak substantially, which is supported by field observations at the McGlave Gas field (Nelson und Simmons 1995), from concentration profiles for light hydrocarbons in commercial size gas-condensate fields in North America (Krooss et al. 1988) and from numerical simulations (e.g., Krooss et al. 1988). There are many examples where gas leaks occurred along faults cross-cutting seals formed by clay shales, such as at the Ketzin gas storage site Germany (Juhlin et al. 2007), the Haltenbanken Province in the North Sea (Vik et al. 1991), and the St. Gallen Geothermal Well in Switzerland.

2.2 The St. Gallen Geothermal Well

There are many examples in the Northern Alpine foreland of Switzerland with substantial long-term gas leaks through the Opalinus Clay (NAB 12-32; NAB 14-70; Schaub 2009, his Fig. 17). The best studied example is the St. Gallen geothermal well drilled into the steeply dipping St. Gallen Fault Zone. A ML 3.5 seismic event during drilling of the geothermal well St. Gallen GT-1 was triggered by the need to increase the density of the drilling mud and therefore increase the pore pressure in response to a gas spike in the fractured Malm (Upper Jurassic) limestones. The borehole was terminated in the very top of the Dogger at 4253 mTVD (Wolfgramm et al. 2015, their Fig. 4). The determined static pressures at the top of the Malm indicate that the gases are stored in a fractured reservoir in the Malm but from the volumes involved, composition (94% methane), and isotopic character, the gas is interpreted to be sourced from a Permo-Carboniferous basin underlying the Mesozoic sequence (Wolfgramm et al. 2015; Heuberger et al. 2016). The amount of gas was such that it was seriously considered as a commercial proposition[1]. This large volume of gas must have migrated from below the Mesozoic section to its current level in the fractured Malm limestones above the Opalinus Clay. In this case, the Opalinus Clay clearly did not act as a continuous and impermeable seal for gas. Although in the current regional stress field the St Gallen Fault zone is a transtensive sinistral strike-slip structure, 3D seismic interpretation indicates that it was a long-lived structure with multiphase tectonic activity from at least the Late Paleozoic to the early Oligocene, or even later (Heuberger et al. 2016). This has resulted in a variable amount of accumulated normal (down-to-the-SE) displacement, which locally can lead to the reduction or even total tectonic elimination of the Mesozoic sequence along individual fault strands (e.g. Fig. 9 of Heuberger et al. 2016). In the absence of clay smear and sealing along such fault strands, such a breach of the Opalinus Clay horizon could potentially explain the observed migration of gas from below the Mesozoic sequence into the level of the Malm limestones.

As established from the geothermal experiment, the St. Gallen Fault Zone is critically stressed and presumably intermittently seismic, even without artificial stimulation. Although generally self-sealing, the Opalinus Clay could also act temporarily as a conduit for gas and fluids during transient seismic or aseismic movement. This is consistent with the observations from the Main Fault in Mont Terri URL (e.g. Guglielmi et al. 2017; Jeanne et al. 2018).

From a joint interpretation of earthquake and seismic data related to seismicity induced by the St. Gallen deep geothermal project, Diehl et al. (2017) show that the majority of the seismicity occurred in the pre-Mesozoic basement, hundreds of metres below the borehole and the targeted Mesozoic sequence. They propose a hydraulic connectivity between the reactivated fault and the borehole, most likely through faults mapped by seismic data. They note that stimulation and clean-out operations in the open section of the borehole at the level of the Malm correlate with almost immediate seismic activity in a cluster below the Mesozoic sequence. They conclude that this temporal correlation between borehole operations and microseismic activity at greater depth suggests a hydraulic connection between the two. They propose that it is possible that the proposed hydraulic connection extends below the activated fault segment and acted as a pathway for the released gas from the postulated Permo-Carboniferous trough. Such an interpretation implies that hydraulic connectivity from the Malm to the Permo-Carboniferous already existed before seismicity and was critical for triggering of seismicity at depth, rather than the other way around (i.e. that the seismicity caused transient hydraulic connectivity). This interpretation, at least for the immediate vicinity of the St Gallen Fault Zone, would contradict the general conclusions of NTB 14-02-V. In that summary of the regional hydrology of the siting regions it was noted that in general faults can be transmissive, leading to hydraulic connectivity between different aquifer levels. However, the important result of this summary was that the hydrochemical data from the various hydrogeological units show that the characteristic differences are undisturbed, especially in rocks underlying the Molasse Basin from northeast of the Folded Jura to the edge of the Hegau-Bodensee Graben. Thus, the deep groundwaters in the Tertiary / Malm aquifer system are chemically different in composition from those in the Keuper and Muschelkalk aquifers. In this tectonically little deformed area, the conclusion of NTB 14-02-V was that an intact layered structure is present, with the low-permeability sequence 'Brauner Dogger' - Opalinus Clay - Lias and the Gipskeuper efficiently separating the Tertiary / Malm-Aquifer, Keuper-Aquifer and Muschelkalk-Aquifer. However, in the case of the St. Gallen Fault Zone, this has locally not been the case, if the interpretations of Diehl et al. (2017) regarding hydraulic connectivity between Malm and basement are correct.

[1] https://www.tagblatt.ch/ostschweiz/stgallen-gossau-rorschach/stgallen-stadt-verzichtet-auf-gasfoerderung-ld.378295

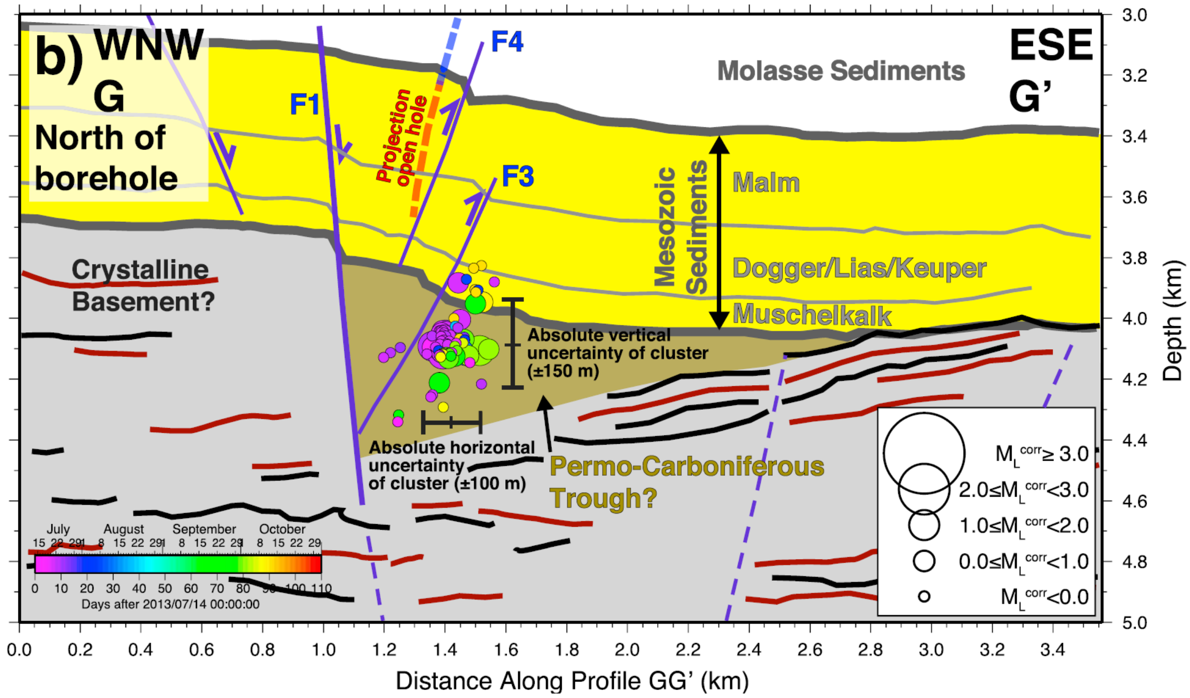

Figure 1: Summary figure with seismicity projected onto reflection seismic profile of Heuberger et al. (2016). Bold black and red lines sketch prominent reflectors identified in the 3-D reflection images of Heuberger et al. (2016). Purple lines mark faults proposed by Heuberger et al. (2016) based on the tracking of vertical offsets in the reflection horizons. F1 is a SE dipping normal fault. F3 and F4 are NW to WNW dipping thrust faults. The activated fault hosting the induced ML 3.5 event is dipping toward NW. From Diehl et al. 2017.

As summarized in Diehl et al. (2017), their Fig. 2, the source region of the induced seismicity related to the St Gallen deep geothermal well either lies below the Mesozoic sequence or straddles the lower boundary of the Mesozoic sequence. The authors conclude that the majority of the induced earthquakes locate in the pre-Mesozoic basement in all their models. However, even in such a well-constrained study, there is a limit to the accuracy of the hypocentral solutions, which they estimate as ±150 m for the focal depth. For a model as shown in their Fig. 2c, a significant number of aftershocks could have a focal depth corresponding to the Opalinus Clay. This is of interest in assessing the potential for seismic slip in reactivated faults within the Opalinus Clay, especially considering the experimental work of Orellana et al. (2018), who found that the scaly clay fabric developed in Opalinus Clay fault zones could have the potential for nucleation and propagation of earthquakes. This could be promoted by rapid loading due to seismic slip propagation from below along pre-existing faults extending from the basement through the Mesozoic sequence, as in Fig. 1.

Although the St. Gallen Fault Zone is currently the best studied example, there are many other examples scattered throughout the Alpine Foreland of gas seepage to the surface (Greber et al. 1995; Schaub 2009; Sachs und Eberhard 2010; NAB 12-32, Beilage 4; NAB 14-70, Fig. 17) or accumulation at levels above the Opalinus Clay (Greber et al. 1995). A significant natural gas seep occurs on the steep NNE-SSW – striking sinistral Sarnen Fault Zone in the Swiss Northern Alps (Etiope et al. 2010), which is seismically active (Burkhard und Grünthal 2009; Fritsche et al. 2009) but was not discernible in a 2D seismic campaign (Ebert et al. 2013). Considering the degree of thermal maturity necessary, the most likely source for the thermogenic gas in all these cases is, as in the case of the St Gallen Fault Zone, established or probable underlying Permo-Carboniferous basins (NAB 12-32; NAB 14-70). The only commercial gas production in Switzerland was from Finsterwald (Entlebuch-1), where the reservoir was (like St. Gallen) in fractured Upper Jurassic (Malm) limestone (Klöckner 1986; Vollmayr und Wendt 1987) and the source is most likely the underlying Permo-Carboniferous basin, which was drilled as far as the Carboniferous (Vollmayr und Wendt 1987). The interpreted seismic cross-section of Transect 08 in Sommaruga et al. (2012) runs NNW-SSE almost directly through Entlebuch-1 and shows a gentle anticlinal culmination but no faults with discernible vertical offset at the location of the well. The nearest SW-NE long-section (Transect 15) crosses Transect 08 some 5 km to the NW and there is no 3D seismic study, so the possible presence and distribution of steep faults related to the “fractured Malm reservoir” of the Finsterwald gas occurrence cannot be critically assessed.

As discussed by Greber et al. (1995) and summarized in their Fig. 6, gas can migrate large distances from source to possible reservoirs or to the surface, utilizing open fault structures and fractures and more permeable rock units, such as porous sandstones or karstified limestones. As summarized in NAB 14-70, the most important structural phases in the Alpine Foreland are younger than the main hydrocarbon generation and migration phases and older structures that have been reactivated tectonically may have lost their integrity as a seal. In this regard, the origin of light hydrocarbons recovered from gases in borehole headspaces in the Mont Terri URL (Pearson et al. 2003, Appendix 8) remains controversial. Pearson et al. (2003) recognized that the thermal maturity of the Opalinus Clay at Mont Terri was too low for an in situ thermogenic origin. They argued instead that light hydrocarbons in the Opalinus Clay were derived by fermentative anaerobic decomposition of the organic material present in the formation. In contrast, NAB 11-33 concludes that the presence of a significant thermogenic component should be considered because there is clear evidence of the presence of such a component. The report infers that the possibility of migration of hydrocarbons from underlying sources (Lias?) has not been considered, but cannot be excluded. Vinsot et al. (2017) more recently also concluded that the relative fractions and isotopic composition of the alkanes extracted from the Opalinus Clay at Mont Terri URL are consistent with the hypothesis of a thermogenic origin.

3. Structure and Fabric of Steep Fault zones in the Proposed Siting Regions

The observations and interpretations of Nagra with regard to the regional distribution of fractures and faults are based on extensive field work (NAB 12-41, with summaries in NAB 14-01 and NTB 14-02-II), together with observations from the Mont Terri Underground Laboratory and more limited data from deep drill holes (Riniken, Benken, Schlattingen-1, etc). In the proposed siting regions, the Opalinus Clay (OPA) occurs at depths of ca. 300-900 m below surface, so it follows that field observations in the siting regions and immediately adjacent areas are restricted to higher units, especially the competent and better outcropping Upper Jurassic (Malm) limestones. As noted in NAB 12-41, the great majority of fractures observed in the field should be classified as "joints", because the offset is either not discernible or at the most small (less than a few cm). However, most (60-80%, NAB 14-01) of these "joints" carry kinematic indicators, indicating that they are not strictly extensional (mode I fracture) but instead are either mode II (shear) or mixed mode (shear + extension) fractures. Most kinematic indicators found on fracture planes suggest strike-slip faulting. The occurrence of reverse faults is mostly limited to high-strain areas affected by the tectonics of the Jura Fold-and-Thrust Belt.

In terms of fracture kinematics (as summarized in NAB 12-41), the potential siting region Jura Ost is dominated by strike-slip faults and less commonly reverse faults. In the region around Nördlich Lägern, strike-slip and reverse faults are also common but here normal faults occur more frequently. Normal faults dominate the easternmost potential site of Zürich Nordost. Strike-slip faults are also commonly found here but reverse faults are absent. These observations suggest differing influences of various tectonic events on the individual siting regions. However, the overall stress tensor interpreted from the measured faults and slip vectors is rather consistent across all the siting regions and is the same as the present day, with the maximum principal compressive stress axis ca. horizontal NNW-SSE (i.e. perpendicular to the Alpine chain) and the minimum principal compressive stress ca. horizontal ENE-WSW (i.e. parallel to the Alpine chain) (e.g. Kastrup et al. 2004). According to Burkhard und Grünthal (2009), the present-day tectonic regime in the potential siting regions is generally dominated by strike-slip faults, with a minor normal fault component and even less potential for thrust development or reactivation (≤ 5%, see their Fig. 6).

When optimally placing the repository within one of the siting regions, the aim is to avoid tectonically disturbed zones, which includes both zones of thrusting related to the Jura Fold-and-Thrust Belt and larger steep faults and fractures. However, steep strike-slip faults with minimal vertical offset are not directly discernible on seismic sections and are therefore more difficult to specifically avoid. Relatively continuous NNE-SSW-striking linear patterns were already recognized in the parameter maps calculated from the 1996 3D seismic data for ZNO (NTB 00-03, e.g. their Fig. 4.11) and interpreted as structural zones without discernible vertical offset – implying that that they were either strike-slip faults or extensional fractures. The N-S to NNE-SSW-striking Effingen and Umiken Faults in the Jura Ost siting region were only more recently identified from 3D seismic interpretation (NAB 18-34), with their probable minimal strike length established based on coherence, curvature and dip seismic attribute horizon slices. The strike of these faults is identical to the most common strike direction of steep faults determined from surface observations throughout the siting regions, namely NS to NNE-SSW with a dominant sinistral strike-slip sense (NAB 12-41; Egli et al. 2017).

In summary, the 3D seismic data (NAB 18-34; NAB 18-35; NAB 18-36) show N-S to NNE-SSW striking features in all three siting regions with extensions of 1 to 10 km. Some of them are not only identifiable in the attribute plots of TLi (Top Lias) and TOp (Top Opalinus) but also in other Mesozoic horizons. In the 1996 3D seismic data of ZNO (NTB 00-03) several features with N-S to NNE-SSW strike have also been identified. Their interpretation as faults with a potential for strike-slip deformation in the current stress field, although with little vertical offset, was provided as an option in NTB 02-03.

A subsidiary maximum in the steep fault orientation that strikes ca. WNW-ESE to NW-SE (e.g. NAB 12-41, their Figs. 4.2-4, 4.2-9, 4.2-16, 4.3-3, 4.3-4, 4.3-15, 4.5-5, 4.5-12) may correspond to a dextral conjugate set. In particular, within the area adjoining ZNO toward the NE, the older Freiburg-Bonndorf-Bodensee fault zone has this general strike orientation and therefore the propensity to be dextrally reactivated in the current stress field (e.g. Egli et al. 2017, their Figs. 12, 16).

As summarized in NAB 14-01, fracture spacing as determined from surface outcrops in all siting regions is approximately 0.5 – 1 m for subvertical fractures and several metres for moderately to gently dipping structures, with generally closer spacing for mechanically more competent and thinly bedded layers (NAB 12-41). However, because the Opalinus Clay is generally subsurface in the siting regions and regionally poorly exposed, there is little direct field data on fault or fracture spacing within the Opalinus Clay itself.

Madritsch and Hammer (NAB 12-41) were careful to point out that their extensive field study was hampered by the outcrop conditions and that the degree of exposure was very different between the three proposed siting regions for SGT Stage 3, precluding a direct comparison. In particular, they note that:

1. the outcrop situation within and around the Jura Ost siting region is very suitable for the investigation of brittle structures;
2. the outcrop conditions within the siting region Nördlich Lägern are unfavourable;
3. the outcrop conditions within the siting region Zürich Nordost are very unfavourable.

The most important (currently known) larger-scale faults in the Alpine Foreland with a NS to NNE-SSW strike, steep dip, and sinistral strike-slip movement sense are the Fribourg Fault Zone or "Fribourg Lineament" (Kastrup et al. 2007; Vouillamoz et al. 2017) and the St. Gallen Fault Zone (Heuberger et al. 2016). Both these faults are seismically active. They transect the whole Mesozoic section (i.e. including the OPA). However, there is no reason why these faults should be unique structures and there is the real potential for many other similar parallel structures, such as the Effingen and Umiken Faults recently recognized in the Jura Ost siting region (NAB 18-34).

Until now, there is no data on the distribution, microstructure and mechanical properties of steep mode II (shear) or mixed-mode (extension + shear) faults within the OPA at the depths of the potential sites. As clearly summarized in Figs. 5.5-4 and 5.5-5 of NTB 02-03, observations from two steep faults in the Opalinus Clay observed in the Benken drill hole and in the Siblingen quarry demonstrate that they are "composite deformation zones", with a broader adjacent damage zone, and thus distinctly different from the "localized deformation zone" typified by the Main Fault in Mont Terri. In the conclusions of NAB 12-41, it was noted that this "comprehensive re-evaluation of the field observations and their kinematic interpretation" could be "considered a valuable data base for the planning and execution of future investigation steps (e.g. quantitative fracture investigation, sampling campaigns etc.)". This necessary additional quantitative information is still lacking. As noted in NAB 14-01, "the key structural databases in the subsurface are boreholes. The near-to-vertical trajectory of deep boreholes in Northern Switzerland implies that subvertical fractures tend to be undersampled."

The processing of results provided by Nagra so far indicates that the distribution and spacing of steep faults are different in the three sites. As these near-vertical faults represent the dominant neotectonic to recent structures and as the tectonic boundary conditions for these structures are different in the three sites, we expect different densities, transmissivities and reactivation potentials. Thus, these faults can be relevant not only from a safety perspective but also for site selection.

The EGT suggests a number of steps that will shed more light on these steep ca. NNE-SSW-striking structures: (1) Reprocessing and evaluation of attributes with state-of-the-art methodologies. This should provide a more objective assessment of differences in the extent and density of these structures in the siting regions. (2) 3D-VSP or Walkaway-VSP measurements in the deep boreholes. This. This will provide information on the reflectivity of the vertical faults in the Opalinus Clay but also in other Mesozoic strata. (3) Drilling of vertical and inclined boreholes that intersect and test a representative number of such faults at multiple scales within the Opalinus Clay. The first two steps can be taken without changing the time schedule for the decision regarding site selection (2022). A program for drilling one or several inclined boreholes is more demanding in this respect and is discussed in Chapter 8.1.

4. Strength, Dilatancy and Criticality of Fault Rocks in the Opalinus Clay

In order to investigate quantitatively the possibility of fault creation, reactivation and gas or brine transport along a fault zone in the Opalinus Clay, mechanical and hydraulic properties of fractures and fault rocks under various loading conditions are required. This Chapter summarizes the current state-of-knowledge of these Opalinus Clay properties. Most available data are from the Main Fault at the Mont Terri Underground Laboratory. As the rock mechanical properties at the siting locations and depths differ significantly from the properties at the Mont Terri Lab, such information can only be transferred under major restrictions.

4.1 Strength and Dilatancy of Mont Terri Rock Samples

Amann et al. (2017) summarize the rock mechanical properties of intact Opalinus Clay samples from Mont Terri under low confining stress (0-4 MPa), i.e. in the repository near field and EDZ. Unconsolidated and undrained compression tests on Opalinus Clay samples (specimens loaded normal to bedding orientation) show that the onset of dilatancy occurs at about 2 MPa differential stress for all tested confining stresses and is associated with the formation of micro-cracks and measurable micro-seismic signals. At differential stress levels above the onset of dilatancy, Opalinus Clay deforms in a highly non-linear manner, yielding long before peak strength. This behaviour can be represented by a bi-linear failure envelope with a high friction angle (43°) and apparent cohesion of 2 MPa at low confinement (<1 MPa), and a very low friction angle (11°) and high apparent cohesion of 4 MPa at higher confinement (1-4 MPa). The amount of dilatancy decreases with confining stress and becomes negligible at effective confining stresses of 4 MPa (Wild und Amann 2018). The strength properties of Opalinus Clay when loaded unfavourably (oblique) to bedding are smaller than the values reported above. Samples from fault rocks show similar properties as bedding planes of intact rocks at residual strength. The shear strength of fault rocks was determined by Haug (2009) between 0.4 and 4 MPa normal stress and fitted to a bi-linear curve with C1=0.1 MPa, φ1=22° (<3 MPa), and C2=0.6 MPa, φ2=11° (>3 MPa).

Wild et al. (2015) performed a series of compression and Brazilian tensile strength tests under variable relative humidity (19-99%) and total suction (0-220 MPa) conditions. The study revealed that suction (or water content below full saturation) has a major influence on the onset of dilatancy, strength and stiffness of intact Opalinus Clay. As shown for example in NTB 08-07, Opalinus Clay shows high capillary pressure (10 MPa) even at high water saturation (>90%). This might have significant influence on the behaviour of galleries in Opalinus Clay, which may be supported by significant apparent cohesion before resaturation.

Orellana et al. (2018, 2019) performed a series of experiments to determine the frictional properties of OPA faults at the Mt Terri URL. For simulated fault gouge, produced by compacting pulverized samples of intact OPA, experiments with normal stresses of 4-30 MPa (corresponding to ~ 100-1000 m depth) and with velocity steps of 1–300 µm/s indicate that the velocity dependence of friction is in the velocity strengthening regime and that zero healing values imply a lack of re-strengthening during interseismic periods (Orellana et al. 2018). Taken together, if an OPA fault reactivates, their experimental evidence favours an aseismic slip behaviour, making the nucleation of earthquakes difficult, with long-term weakness resulting in stable fault creeping over geological times. In contrast, scaly clays with anastomosing polished surfaces, which can be formed experimentally in OPA at low normal stress (≤20 MPa) and at sub-seismic velocities (≤300 µm/s), show a velocity-weakening and -strengthening behaviour, low frictional strength, and poor re-strengthening over time, conditions required to allow the potential nucleation and propagation of earthquakes (Orellana et al. 2018). Orellana et al.

(2019) contrasted the mechanical and hydraulic properties of wet and dry fault zones in OPA, presenting a systematic laboratory study on the frictional strength, stability, dilatancy, and permeability of simulated Opalinus Clay gouge under typical repository conditions. They concluded that wet gouges exhibit an extremely low coefficient of friction ($\mu_f \sim 0.16$), velocity-strengthening behaviour, shear-enhanced dilatancy at the onset of slip, and permeability increase. Conversely, dry gouges remain weak ($\mu_f \sim 0.36$) but exhibit a transition from unstable to stable sliding with increasing sliding velocity. Thus, they infer that faults hosted in OPA could be easily reactivated via aseismic creep, possibly acting as poor fluid conduits. However, if temporarily dried, the faults become potentially unstable, at least, at low sliding velocities (< ~10 µm/s).

All lab tests reported above refer to short term strength and deformability behaviour. At the same time many studies have shown that strength and deformability are time-dependent (Hoek und Brown 1980), and many rocks fracture already below peak stress as determined in classical compression tests (Damjanac und Fairhurst 2010). In brittle rocks this subcritical crack growth is influenced by strain rates and stress levels (relative to peak), as well as by chemical conditions, saturation and temperature (e.g. Paraskevopoulou et al. 2017; Paraskevopoulou et al. 2018). *Loading of the repository near-field by gas pressure is a long-term process, and a better understanding of the long-term strength and deformability of the brittle-ductile Opalinus Clay is potentially also a key behavioural aspect for long-term safety.*

4.2 Fault Slip at Mont Terri

Faults within the OPA can be observed in various quarries, boreholes and in the Mont Terri Underground Laboratory (URL) (NAB 14-01). However, research to date on fault geometry, microstructure, porosity, permeability and potential for reactivation within the OPA has been concentrated on the Mont Terri URL, and especially the "Main Fault". The Mont Terri URL Main Fault is a higher order splay from the main thrust surface that has been steepened in the back limb of the Mont Terri anticline (to a dip of ca. 45°, e.g. Laurich et al. 2018, their Fig. 1). As a result, it is now unfavourably oriented for reactivation, either as a thrust or strike-slip fault (e.g. Vouillamoz et al. 2017). It is important to note that Nussbaum et al. (2011) specifically state "the tectonic setting and structural geology of the laboratory, as described in this paper (e.g. fracture frequency, fracture sets), is not representative of the potential disposal sites located in the north-eastern part of Switzerland".

There are no studies of gas flow in faults or gas induced fault reactivation in Opalinus Clay. The most detailed investigation of slip and fault leakage in fully saturated Opalinus Clay, is the Fault Slip (FS) Experiment carried out in Mont Terri in Fall 2015 (Guglielmi 2016). The Fracture Opening Pressures recorded in the Main Fault of the Mont Terri laboratory vary between 3.9 (+/- 0.1) and 5.3 MPa. This value corresponds to 50-75% of the vertical stress at the test location in Mont Terri, which is around 7 MPa (Guglielmi et al. 2017). The minimum Fracture Pressure at the Onset of Leak-Off as determined during the FS experiment ranges between 1.89 (+/- 0.1) and 3.5 (+/- 0.2) MPa, and therefore corresponds to 25-50% of the vertical overburden stress.

The recorded displacement vectors of the FS experiment, when projected on the reactivated fault planes showing similar strike/dip orientations (039-058º/59-69ºE), show dilatancy and display significant variations in mode and directions within this complex fault zone. These variations are explained by local stress variations within the fault zone. The small fault slips (sub-millimetre) of these experiments lead to a 5-6 order of magnitude transmissivity increase on a critically stressed 30-50 m^2 patch of the fault core-damage zone interface. Back-calculated friction coefficients of slipped patches are very low and range between 0.2 and 0.3 (Guglielmi et al. 2015; Jeanne et al. 2018).

Contrasted fault movements were observed, mainly dilatant in the fault core, highly dilatant-normal slip at the fault core-damage zone interface, and low dilatant-strike-slip-reverse in the damage-to-intact zones (Guglielmi et al. 2017). Jeanne et al. (2018) note that because rupture may in certain cases destroy permeability, this succession of ruptures may not necessarily create a continuous hydraulic pathway. The stress field in the Mont Terri URL is uncertain. Martin und Lanyon (2003) consider σ1 to be nearly vertical, which is not typical of the current regional stress field in the Alpine Foreland (Kastrup et al. 2004). The minimum compressive stress is considered to be nearly horizontal and NE-striking. This is typical of the regional stress field, but the reported magnitude is remarkably low (≤~1 MPa; Martin und Lanyon 2003), so that a direct application of results from Mont Terri URL to the OPA at depth in the siting regions is questionable.

The connectivity of the observed enhanced porosity and permeability / transmissivity during transient fracture reactivation of the Fault Slip experiment at Mont Terri is crucial for the overall self-sealing properties of Opalinus Clay. As noted in Jeanne et al. (2018), similar ruptures can create or destroy the fluid diffusion pathways and a succession of ruptures may not necessarily create a continuous hydraulic pathway. Slickensided shear surfaces from the Main Fault in Mont Terri show a strong preferred orientation of clay minerals, a very marked reduction in porosity, evidence for neocrystallization of clay minerals (illite), and re-establishment of a low permeability comparable with the original Opalinus Clay (Nussbaum und Bossart 2008; Laurich et al. 2014; Laurich et al. 2018). However, the growth of calcite and celestite along the fault surfaces indicates periods of transient higher permeability and fluid advection during thrust movement. Based on isotope profiles (Sr, S, O, C), de Haller et al. (2014) suggested that Opalinus Clay acted as a seal for fluid flow during most of its history except during the movement of the Main Fault. These isotope data suggest that veins formed during a single geotectonic event that allowed fluids to flow across the Opalinus Clay, with the main fluid source located in the underlying Trias. Petrographic data combined with structural information indicate that vein mineral precipitation was syntectonic and most likely occurred during the Jura folding and thrusting.

4.3 Criticality of Opalinus Clay Faults in the Alpine Foreland

Opalinus Clay from potential siting areas in Northern Switzerland has different strength and dilatancy properties than the samples from Mont Terri, due to regional variations in burial and uplift history (over-consolidation), diagenesis, repository depth and lithology. Hydro-mechanically coupled triaxial tests on Opalinus Clay from Mont Terri show that the effective consolidation stress (i.e. the degree of over-consolidation) has a major impact on the sample dilatancy during differential loading. More details are given in Wild und Amann (2018). Samples from the siting regions tend to be stronger than from Mont Terri, but a detailed characterization is pending and a focus of Stage 3 of the SGT.

Away from zones directly related to the Jura Fold-and-Thrust Belt, the current regional stress field in the Alpine Foreland, which has been active since at least the early Miocene, is one conducive to steep strike-slip faulting (Kastrup et al. 2004). In their study of the Fribourg Lineament (FL), which is one of the most important of these strike-slip fault zones (Kastrup et al. 2007), Vouillamoz et al. (2017) note that deformation due to NW–SE directed compression of the northwestern Alpine foreland of Switzerland preferentially manifests itself as slip on favourably oriented strike-slip/tear faults rather than on favourably oriented thrust/reverse faults, because the differential stress needed to activate a thrust fault is significantly higher than for a more or less vertical strike-slip fault at the same depth (Sibson 1974). Thus the existence and repeated rupture of favourably oriented critically stressed tear faults, such as the N–S oriented fault segments that constitute the FL, sets a limit to the magnitude of the ambient differential stress. As a consequence, the differential stress cannot reach a sufficiently high level to activate any possibly well-oriented reverse faults. These authors note that critically stressed faults are also generally hydraulically conductive faults (Townend und Zoback 2000), supporting the idea that seismically activated zones typically act as active fluid conduits.

The other known major steep fault in the Alpine Foreland is the St. Gallen Fault Zone (SFZ), whose critical state of stress and propensity for seismic reactivation was unwillingly tested during drilling associated with a deep geothermal project (Chapter 2). The fault zone strikes NNE–SSW and dips steeply to the SE (Moeck et al. 2015; Heuberger et al. 2016). As summarized by Moeck et al. (2015), the regional stress field is typical of the Alpine Foreland (e.g. Kastrup et al. 2004) and corresponds to a strike-slip regime, with the maximum horizontal stress SH trending NNW-SSE (160±12°). The St. Gallen Fault Zone shows evidence for multiphase tectonic activity from at least the Late Paleozoic to the early Oligocene, or even later (Heuberger et al. 2016), but has now been reactivated as a mixed-mode (dilation / extension + shear) sinistral strike-slip structure, with a possible critical fault stress state under transtensional stress regime conditions (Moeck et al. 2015). This transtensional stress state was confirmed by seismic events triggered by the drilling (Moeck et al. 2015). As noted by Heuberger et al. (2016), most faults constituting the SFZ are favourably oriented in the present-day stress field to be reactivated in strike-slip mode. Even though the seismicity of northeastern Switzerland is considered to be low and diffuse, parts of the SFZ have to be regarded as critically stressed (Heuberger et al. 2016).

In summary, both the major steeply dipping N-S (Fribourg Lineament) to NNE-SSW (St. Gallen Fault Zone) -striking fault zones are currently critically stressed and intermittently seismically active in a transtensive sinistral strike-slip regime. Both potentially root into the basement (Kastrup et al. 2007, Heuberger et al. 2016) or at the least into weak evaporite-rich layers within the Triassic (Vouillamoz et al. 2017) and thus transect the OPA. Similarly oriented faults and fractures within the siting regions (e.g. the Effingen or Umiken Faults in Jura Ost) are expected to also be potentially critically stressed, with the potential for dilatant sinistral strike-slip movement and associated enhanced transient permeability during seismic or aseismic reactivation.

Only very few experiments have investigated fault strength properties of Opalinus Clay, especially considering the stress and consolidation history in the repository siting regions. In addition, Opalinus Clay shows a strong dependence of its strength and stiffness properties on saturation, and it is expected that fault reactivation in Opalinus Clay by gas pressure build-up cannot be adequately assessed from fully saturated experimental conditions. This also holds for fault zones, where pore sizes and fracture apertures require capillary forces to be considered. It is therefore recommended to investigate fault rock strength properties and conditions for fault reactivation under fully saturated and partially saturated conditions with specific lab and field experiments.

5. Gas production in the HLW and L/ILW Repositories

Nagra discusses gas volumes, gas generation and consumption processes as well as respective reaction rates in a number of reports and publications for different HLW and L/ILW repository scenarios. In general, gas generation mechanisms are more complex in L/ILW than in HLW repositories. Due to the complex composition of waste inventory in the L/ILW, including significant amounts of organic matter, various gases can be generated by abiotic and microbially induced processes. Corrosion of metallic components of concrete reinforcement and predominantly the waste container walls is the main source of gas evolution in a HLW repository. Despite the different waste composition of HLW and L/ILW, H_2 generated by metal corrosion represents the main gas volume component in both repositories.

In the following we will first summarize the gas production rates as presented by Nagra (Chapters 5.1 and 5.2, and then evaluate and discuss these results (Chapter 5.3).

5.1 Gas Production in the HLW Repository

According to Nagra (i.e. NTB 16-03), inflowing host rock porewater will saturate the bentonite buffer after closure of the repository within several hundred years. As a consequence of swelling and host rock convergence, the full pressure (swelling pressure plus pressure due to convergence) will be reached in the repository within this time period (NTB 02-05, p.132). Early gas evolution might be due to corrosion of rails and reinforcement components, while container corrosion will start when buffer saturation progresses and water reaches the container wall surface. Nagra assumes in its considerations that H_2 evolution from corrosion of all metallic components starts immediately after repository closure. Steel corrosion rates are taken as 2 µm/a for the «base case» where a variation in a range of 0.1 – 5 µm/a is considered in sensitivity analyses (NTB 16-03, Tab. 2-2). As a result, a more or less constant annual H_2 production rate per m of disposal drift of < 2 x 10^{-2} m^3/m*a («base case») is derived due to abiotic iron corrosion. Microbially induced corrosion (MIC) is considered irrelevant as the pore volumes at the container wall/compacted bentonite interface will be too low to allow bacteria to grow (NTB 08-12). Taking the thermal phase in the repository near-field into account, a pressure maximum due to gas evolution processes is reached after about 500 years. Considering the corrosion rates, thick walled carbon steel containers will remain integer for about 10,000 years, so that radionuclide release via gas transport must not be considered during the high gas pressure period. When the container breaches and water accesses the inner parts of spent nuclear fuel (SNF) containers, relatively rapid corrosion of aluminium and zinc components induces a second pressure increase. Assuming a rapid corrosion for those base metals is reasonable, despite rate data for the corrosion of those components under relevant conditions are rarely found in the literature (e.g. Delaunois et al. 2014). During this phase, a potential radionuclide release has to be taken into account.

Clear reduction of gas evolution can be achieved by replacing or covering carbon steel containers by corrosion resistant containers e.g. made of copper or copper coated steel comparable to the Swedish KBS-3 concept (NTB 16-03, p. 84, Fig. 4-7).

5.2 Gas Production in the L/ILW Repository

Gas evolution in an L/ILW repository is assumed to start immediately after waste emplacement (NTB 16-03, Chapter 3). Cemented waste already contains water, so that corrosion processes start early. Abiotic and microbial processes result in the generation of various gases (H_2, CO_2, CH_4, H_2S, NH_3 etc.), where H_2 represents by far the largest contribution to generated gas volumes. Metal corrosion rates in the L/ILW facility are considered lower than under HLW repository conditions. Respective metal corrosion rates in the high-pH cement pore waters are taken at 0.02 µm/a («base case»; NTB 16-03, Tab. 2-2) and are comparable to values recently determined for conditions relevant for the Belgian supercontainer concept, where an overpack made of concrete is foreseen for HLW disposal (Smart et al. 2017). However, the surface area of metallic waste components is larger than the surface area of HLW containers. H_2 production rates can, thus, be higher than those in the HLW repository by orders of magnitude.

To limit and control (engineer) gas pressure build-up in the repository, Nagra proposes the implementation of an Engineered Gas Transport System (EGTS)[2], consisting of porous bentonite/sand mixtures and gas permeable seals (NTB 08-07). Geochemical reactions and notably the precipitation of secondary solid phases (primarily Calcium Silicate Hydrates) at the interface between the cementitious material in the emplacement caverns and the backfill material of the EGTS drift may lead to clogging and to an at least partial loss of gas permeability in the EGTS (see NAB 14-16 and references therein). Calculations suggest that the porosity in the bentonite/sand under extreme conditions decreases by about one third (NTB 08-07). Kosakowski and Smith (NAB 14-16) propose in addition separating the cement based medium and the bentonite/sand backfill by a layer of calcareous sandstone gravel. As a result of THMC calculations, precipitates will then form spatially distributed, significant pore clogging will be avoided and gas permeability will only negligibly be affected.

Volumes of microbially generated H_2 are hard to quantify due to the strong dependence of gas volumes on evolution and consumption reaction rates. These rates are difficult to assess, as the distribution of different waste components and materials in the emplacement caverns is highly heterogeneous. Under the hyperalkaline cement porewater conditions microbial activities are in general considered low. However, sulfate reducing bacteria may colonize in the porous EGTS medium filled with porewater of lower pH and may contribute to H_2 consumption. Mass balance calculations reveal that sulfate mineral abundance will not be high enough to consume significant amounts of H_2. In order to promote significant microbial H_2 oxidation, sulfate must be added to the backfill material (NTB 16-03, p. 22). Degradation reactions and rates for different low and high molecular weight organic matter and their bandwidths are discussed based on available literature data. Respective reactions are strongly coupled with the abundance of microbial activity and depending on the local heterogeneity of the emplaced waste composition. Quantification of rates is, thus, complex and still subject of ongoing research (e.g. Kuippers et al. 2015; Small et al. 2017; Vikman et al. 2019). Gaseous products of organic matter degradation such as CO_2 und H_2S are reactive and will be bound as $CaCO_3$ and FeS in the near-field of the backfilled emplacement caverns and, thus, do not or only negligibly contribute to pressure build-up (NTB 16-03, p. 22).

Significant reduction of gas evolution by treatment of the waste is not to be expected. Thermal treatment can remove organic constituents but does not significantly reduce gas production. Melting of metallic components offers the potential of reducing their reacting surface area. Respective simulations show that H_2 gas volumes in this case can be reduced by about a factor of 2 (NTB 16-03, p. 39, Fig. 3-8).

[2] The EGTS is the total of all branch and access tunnels that are backfilled with a clay based material (e.g. processed excavated Opalinus Clay, Friedland Clay, sand/bentonite mixtures). This includes different types of plugs in the HLW and L/ILW waste repository. The EGTS is part of the Engineered Barrier System (EBS).

5.3 EGT Evaluation

Nagra's input parameters for the assessment of gas pressures in both repository types concerning corrosion rates, gas evolution and consumption rates are sound and in agreement with the state-of-the art of knowledge in the literature. Respective values fit well into the range of parameters assumed in other radioactive disposal programs (see e.g. De Combarieu et al. 2007). Sensitivity analyses are performed by extensive parameter variations (NAB 16-07, NAB 16-08 and NAB 17-08) and show the robustness of the concept. The assumption that MIC is of minor importance for the long-term container corrosion in the HLW repository appears justified. Féron und Crusset (2014) describe that MIC can significantly induce pitting corrosion during the period where the bentonite buffer is only partially saturated and residual O_2 is present. However, such processes will be relevant for a limited period of time only and will have an insignificant impact on the long-term integrity of the container.

Thermal impact on processes in the L/ILW is not considered by Nagra (NTB 16-03, p. 25). In case of co-disposal concepts, the thermal field of the HLW repository may induce a temperature increase in the L/ILW facility. Respective consequences on gas evolution scenarios should be discussed. While the abiotic anaerobic corrosion of iron is found to be less temperature dependent (e.g. Féron und Crusset 2014), this is different for degradation of organic components and microbially induced processes. Potential consequences of thermal effects on gas evolution in L/ILW evolution scenarios for co-disposal concepts should be discussed.

6. Gas Transport and Pore Pressure Build-up in the Opalinus Clay

6.1 Gas Transport and Pore Pressure Simulations

The scenarios of particular interest to Nagra are gas pressure build-up and induced pore water displacement from the repositories through intact Opalinus Clay, excavation disturbed zone and sealed access drifts. Therefore, the intact host formation has been characterized by Nagra with respect to gas flow and in the presence of water with respect to two-phase flow. The relevant and practically feasible scale of mathematical-numerical description of gas migration processes is the macro scale, often denoted also as Darcy scale or REV scale. On this scale, the classical gas-related properties include porosity, intrinsic and saturation-dependent relative permeability, saturation-dependent capillary pressure). Porosities and permeabilities are strongly coupled to each other while these relationships are, although relatively simple, often very uncertain (e. g. Hommel et al. 2018). This is in particular true for fractured media with fractures or micro-cracks on a scale below the REV-scale. As is elaborated in the appendix (Report R. Johns, items 2, 16 and 18), the complexity introduced by sub-REV-scale micro-cracks requires appropriate methods for an effective up-scaled description. While, theoretically, the concept of dispersion is appropriate, it brings along difficulties in determining dispersivities and distinction of physically motivated dispersion and numerical dispersion. The effects of micro- and macro-cracks on diffusion and multiphase flow have not been considered by Nagra.

The transport processes considered in the simulations of Nagra include essentially advection due to pressure gradients and buoyancy, as well as diffusion with Darcy's and Fick's law as classical and established concepts. Impacts of osmotic pressures and bacterial growth with effects on altered hydraulic properties have not being taken into account (appendix, item 23). Any clogging by bacteria would likely reduce permeability and would cause greater pressure build-up during hydrogen generation. Such scenarios are potentially more relevant for L/ILW at the interface to the EGTS. For rock formations like the Opalinus Clay, an overlapping of Fickian and Knudsen diffusion may take place under certain conditions (see Firoozabadi 2015, Helmig 1997). Nevertheless, recent studies on the influence of Knudsen diffusion (Schaefer und Thess 2019, however in another context), let us assume that at high gas pressures, this is likely to be not important, while at low gas pressures, the flow in very small pores in clay might show a deviation from Darcy's law which would be adequately described by Knudsen diffusion.

Various experimental studies related to the quantification of gas diffusion in saturated clay rock (Boom Clay, Belgium: Ortiz et al. 2002; Jacops et al. 2017; Jacops et al. 2015; Opalinus Clay, Switzerland: Vinsot et al. 2014) are available. In the latter study, the authors determined effective diffusion constants for He, Ne and H_2 in Opalinus Clay directly. Nagra took a value for H_2 diffusion for their calculations (8.3×10^{-11} m^2/s in NTB 04-06) which closely corresponds to the constant determined by Vinsot et al. (2014) within the Hydrogen Transfer (HT) in-situ experiment at the Mt Terri laboratory (8.12×10^{-11} m^2/s). In all studies, H_2 consumption is observed, most likely due to microbial activities (see discussion in Chapter 5 for the situation in the HLW and the L/ILW repository case). By comparing transport capacities for different pathways, diffusive transport of dissolved H_2 is considered negligible (NTB 04-06, p. 50).

Molecular sorption of H_2 onto clay samples including natural Callovo-Oxfordian clay has been experimentally investigated by Didier et al. (2012) and Bardelli et al. (2014). Up to 0.1 wt% of H_2 could be found adsorbed to dry rock samples at room temperature and 40-60 bar. Experimental conditions in their studies are, however, not representative of conditions in a repository.

Sorption competition by water needs to be taken into account, which is expected to counteract H_2 sorption. Therefore, Nagra regards retention of H_2 at clay mineral surfaces as of less relevance. Neglecting sorption to the rock matrix can be justified as a conservative assumption for predicting gas migration (see NAB 13-83, p. 7). Sorption of gas to the matrix could change the multiphase flow behaviour in a sense that it retards gas flow, but it may also lead to apparently increased capillary pressures. Both would impede gas flow. Truche et al. (2018) report in their recent study, that radiolytically generated, natural H_2 is accumulated in clay-rich rocks overlying the uranium ore deposit at Cigar Lake (northern Saskatchewan, Canada). H_2 is found enriched up to 500 ppm (i.e. 0.25 mol kg^{-1} of rock). This seems to be the first work where H_2 sorption in water saturated clay rock is stated. The authors identify sudoite, an Al–Mg di-trioctahedral chlorite, as a main contributor to binding H_2. It might be worth evaluating the consequences of H_2 sorption in repository evolution scenarios on gas pressure build-up in the Swiss concept.

The flow behaviour of gases in previously saturated clay formations is usually influenced by the mobility ratio M and the ratio of capillary versus viscous forces, expressed by the capillary number Ca. The NAB 13-83 report refers to the schematic of Lenormand und Zarcone (1989) with respect to the major flow regimes in the Ca-M space. Under the prevailing conditions in Opalinus Clay, capillary fingering is in many instances the dominant flow regime. While the Lenormand-classification is very common and justified, we note here that ongoing (and unpublished as of late 2019) work of Steeb and Karadimitriou at the University of Stuttgart also investigates the influence of topology on the gas-water displacement processes. Their preliminary experiments on the micro-pore-scale show that there are still uncertainties unaccounted for in current theories.

We consider capillary fingering as not trivial to upscale to the Darcy scale, on which the models usually are conceptualized (see e. g. Lenormand und Zarcone 1989 and NTB 16-03). Therefore, percolation models based on high-resolution imaging methods are required to allow predictive simulations for gas transport invasion patterns. Of course, this is currently not pragmatic for the large scale (the scale on which NTB 16-03 simulations were carried out), and therefore pore-scale details will likely not be represented. But it shows the need for a thorough characterization of the host rock, i.e. the Opalinus Clay, in order to estimate the relevance of preferential migration paths based on knowledge about the orientation of connectivity of macro-pore networks, in particular this refers to potential fractures in the structures (cf. Yang et al. 2019).

Stochastic methods are here a possible way to improve confidence. From the Nagra reports, e.g. NAB 13-83, one can note that perpendicular to the bedding planes, the networks seem to be poorly connected, which is the reason for a rather strong anisotropy. The pore space is formed by a network of mainly micro- to meso-pores in the order of 1-100 nm, thus very small (see e. g. Blunt 2017). Furthermore, some samples, for example Benken, when compared to others like Mont Terri, are more compacted than others, so the majority of pores is classified as meso-pores. Therefore, invasion models based on percolation approaches, e. g. Hunt und Sahimi (2017), under consideration of geostatistical information might improve the process understanding further.

In intact Opalinus Clay, deformation may also play an important role in affecting gas flow by the pressure-induced development of flow paths. Dilatancy-controlled flow is a particular problem for clay or argillaceous porous media with low tensile strength, e. g. Shaw (2015). We consider the available concepts that try to address pathway dilation as rather phenomenological. Few concepts are really convincing at present in the sense that they allow realistic and reliable predictions. An interesting approach is described e.g. in Rozhko (2016). Therefore, these empirical factors and parameters used in the equations as, for example, explained in Sec. 2.2.3 of NAB 13-83 might be associated with an uncertainty that is hard to assess. As stated in the appendix (item 4), the application of coupled flow and geo-mechanical models might help in understanding the relevant mechanisms better. However, such models are still not the established state of the art. Current or recent work (e. g. Beck 2019, Rinaldi et al. 2014, Rutqvist et al. 2012, Both et al. 2017) has introduced models that use explicit and implicit coupling strategies. In order to be applied beneficially in the current context of Nagra, it first requires investigations as to whether or not the physical features induced by dilation can be distinguished from coupling errors of available multiphase flow-geomechanics models.

For fractures, the entry pressure will be in general much lower than in homogenous porous media. We note again that macro-pore network connectivity is a very important information to upscale if possible to the Darcy scale (Nuske et al. 2010). Furthermore, microscale fractures are being generated during the pathway dilation process and macroscale fractures that may already be present (or might form when fracture pressure is exceeded) will likely form the preferential and faster flow path for gas (see Jakobs 2004). As fractures and steeply dipping fault zones are considered very relevant, it is necessary to analyse their properties and impacts on two-phase flow and pressure build-up in more detail than has been done in the available Nagra studies.

The scenarios summarized e.g. in NTB 16-03, can be considered as reasonable simulation studies for intact Opalinus Clay, given the spatial and temporal scales addressed and the currently established state of the art modelling approaches on such scales. The results of the simulations give numbers on the migration of gas within the model domain over thousands of years, with gas release paths mainly from the tunnels and the excavation disturbed zone to the surrounding host rock. We note that this is an REV-scale model and may be not be very predictive with regard to gas flow. The simulated gas pressures stay below the Nagra's safety indicator criteria, which are discussed in Chapter 7. Thereby, two pressure peaks have been distinguished originating from generated heat after a few hundreds of years and from corrosion after breaching of the canisters at around 10,000 years. Gas pressure induced water flow, as modelled by Nagra, also stays below the safety indicator criteria with the flow direction changing over time back and forth due to changes in the pressure fields.

Report 16-03 summarizes the results from sensitivity studies on gas transport and pressure built-up in the HLW (NAB 14-10, NAB 16-08) and L/ILW (NAB 16-07) repositories. What is not discussed is the influence of the constant-pressure boundary conditions assigned to the top and bottom boundary of the 2D model domain which was not varied in thickness. This can limit the pressure peak which is developing when the gas is generated. The simulated pressures strongly depend on the assumed gas production rates, repository depth, and permeabilities of the intact Opalinus Clay, and seals of the "Engineered Barrier System" (EBS). The sensitivity runs give plausible estimates of expected maximum pressures and brine flow rates, assuming the parameters and processes selected by Nagra are applicable. However, the reliability of some of the parameters and conceptualizations at site scale have been questioned. While some of these processes lead to a likely increase of simulated gas pressure build-up (e.g. bacterial growth), others are supposed to reduce gas pressure (e.g. gas diffusion in micro- and macro-cracks and gas adsorption).

In addition, Nagra is not addressing gas flow and brine transport through fault zones, and the coupled interaction of flow (properties) with geomechanical processes, which are considered very important. We note that predicting the development of pressures for given source terms and permeabilities is much simpler than predicting their consequences in terms of rock damage or the development of preferential flow paths, etc. The prediction of pressure requires mainly a thorough characterization of the overall flow resistance, while prediction of gas flow requires much more local information on heterogeneity, anisotropy, etc.

6.2 Model Input Parameters

Nagra report NAB 13-83 documents a comprehensive set of experimental studies in the field and in laboratories, from which a substantial data base can be derived. This data base includes porosities, intrinsic permeabilities, capillary-pressure curves, relative permeability curves, and critical pressures for the on-set of pathway dilation (see NAB 13-83 und NAB 15-06). Classical capillary-pressure and relative-saturation relationships concepts like the van Genuchten model were originally developed for soil (sand), but not for consolidated rocks and in particular not for tight rock. It is necessary to check the chosen pc-S models and parameterizations in detail, especially with respect to the definition of the entry pressure and the residual saturations (see appendix, items 9-13). There are two papers which might be looked at in this context. Nojabaei et al. (2013) showed for hydrocarbons in tight rocks that the influence of very small pores should not be neglected since their immensely high capillary pressure affects the phase transfer between gas and liquid. This issue might be less important for OPA repository studies than for hydrocarbons with condensible gases. The second paper by Ippisch et al. (2006) deals with the validity limits of the van Genuchten-Mualem model and addresses in particular the issue of not explicitly considered entry pressures in the van Genuchten approach. We recommend assessing in detail whether the usage of van Genuchten models in Nagra's studies can be assumed as conservative.

Core samples from a borehole in Schlattingen (SLA-1) were analysed in the laboratory to determine permeabilities for water and air as well as their dependence on stress-strain conditions. Basically, two different experimental methods were used. Due to fluid flow between samples and walls, Oedometer tests seem to be very difficult to control when the samples have a very low permeability. This is confirmed in the Nagra study NAB 15-06, where reliable results for both air and water permeability could be obtained only in the experiment that used isotropic loading. The experimental protocols, the geologic environment of the samples and their initial conditions before being taken to the lab, the determination of pore-size distributions and water retention curves are well documented.

Nagra report NAB 13-83 refers to a comprehensive set of experimental studies on undisturbed Opalinus Clay. An important note is that for fractures the entry pressure will be in general much lower than in homogenous porous media. Healing of fractures is expected to occur through geological periods of time, but short-term healing mechanisms are poorly constrained. Because fractures or fault zones are relevant in the Opalinus Clay, it is necessary to analyse these two-phase flow properties and stability of fracture and fault rocks in more detail than done in previous Nagra studies. We note again that macro-pore network connectivity is also a very important information to upscale to the Darcy scale (Nuske et al. 2010). Furthermore, microscale fractures that form during the process and macroscale fractures that may already be present (or might form when fracture pressure is exceeded) will likely form the preferential and faster flow path for gas (see Jakobs 2004). With respect to the consideration of heterogeneous rock properties, there are significant uncertainties and it requires case-specific and question-specific investigations, some scenarios requiring different degrees of complexity than others. While for the estimation of pressures, the assumption of homogeneous geologic environments may be reasonable, this is definitely not the case for transport simulations, which are very strongly dependent on the individual development of flow paths.

In-situ hydraulic tests at Mont Terri show that the variations in the very low hydraulic conductivities in the Opalinus Clay are rather limited and expressed in values ranging between $5x10^{-12}$ to $1x10^{-14}$ m/s. However, faults in the potential siting region are expected to be critically stressed (Section 4.3) and fault reactivation leads to an initial 5-6 order of magnitude transmissivity increase (Section 4.2). Gas entry pressures of Opalinus Clay under in-situ conditions range between 1 MPa at Mont Terri and 10 MPa at Benken (NTB 04-06), and are dependent on consolidation history, stress and permeability. Strong local and regional variations in gas entry pressures are expected to occur. Pathway dilation as investigated by Marschall et al. (2013) occurred at Mont Terri at 2-3 MPa below hydrofrac shut-in pressure (minimum principal stress level), and in the Benken borehole (in a fault) at 3-4 MPa below the minimum principal stress (Nagra 2002).

With respect to the consideration of heterogeneous rock properties, there are significant uncertainties and it requires case-specific and question-specific investigations, some scenarios requiring different degrees of complexity than others. While for the estimation of pressures, the assumption of homogeneous geologic environments may be reasonable, this is definitely not the case for transport simulations, which are very strongly dependent on the individual development of flow paths.

6.3 Recommended Supplementary Investigations

There are different challenges associated with modelling gas-related processes in HLW and I/LLW repositories. We think the most basic challenge is to describe the relevant processes on the appropriate scale. While a model formulated on the Darcy scale (or REV scale) in the foreseeable future may be the only feasible and pragmatic option for simulations on the spatial scale of a repository and the time scales required according to the safety regulations, it is rather the pore scale on which the relevant features need to be better understood. As we have pointed out above, the conditions in clay favour in many instances the dominant flow regime of capillary fingering, which essentially occurs on the pore scale and depends on the connectivity of pores. Therefore, percolation models, e.g. pore network models (see Blunt 2017), are likely a required complementary tool to Darcy-scale models in order to address, evaluate, and better understand gas transport mechanisms, although a deterministic approach is not constructive. An investigation on the validity limits of the van Genuchten-Mualem model for the conditions in Opalinus Clay as also recommend by R. Johns (appendix) is considered urgent (see, e. g. the paper of Ippisch et al. 2006). Geostatistical descriptions of pore-scale variations of gas-transport parameters might be an approach that could be pursued in further detail and beyond the sensitivity studies described in NAB 14-10. Furthermore, more experiments and numerical simulations should be done that couple geo-mechanics to non-isothermal flow and transport. Since, as explained further above, such coupled models are still new, there is a strong demand for appropriate benchmark problems that allow the identification of the model error. Since Nagra has to deal with all non-standard aspects of flow coupled to geomechanical responses, at least as long as their negligence is not conservative, the differences in considering a physical detail (in comparison to neglecting it) might be small relative to coupling errors. Therefore, benchmark problems need to be developed specific to the research question, ideally supported by well-controlled experimental evidence.

One may then conclude based on the current state of work that case-specific benchmark exercises would be a good strategy to reduce at least the uncertainty in the numerics where different codes and models are coupled. There are recently some model approaches developed for coupled flow and geomechanical processes (Beck 2019, Rinaldi et al. 2014, Rutqvist et al. 2012, Both et al. 2017) such that this major source of uncertainty could be reduced or minimized.

Therefore we recommend four important fields of further analysis: (i) Finding further experimental evidence on the connectivity of pores and microcracks under changing mechanical, hydraulic, and thermal conditions to identify major factors of influence for a suitable parameterization to be used in predictive numerical simulation models, (ii) improving the understanding of flow regimes from Lenormand und Zarcone (1989), (iii) investigating the two-phase flow *conditions of macro-fractures and fault zone, and (iv) testing percolation models for a more realistic description of capillary fingering regimes. This will require including stochastic approaches to complement deterministic simulations in an appropriate way, aiming at quantifying the uncertainties arising from unknown details and variability of sub-REV-scale pore connectivity.*

7. Gas related Post-Closure Safety Functions and Evaluation Criteria

In the Swiss and Swedish terminology, the performance of repository safety functions is measured with indicator criteria. These criteria are supposed to reflect the conditions under which adverse conditions and safety consequences could be excluded or are expected to arise. If the criteria are not met, or if the criteria cannot be reliably assessed, then detailed investigations of the consequences will be carried out, based on radionuclide release and transport simulations (NTB 14-14). These quantitative assessments should consider site-specific properties (for example gas-entry pressures), their spatial variations (for example due to variations in burial history and porosity), future changes (for example stress state) and uncertainties (for example due to geological heterogeneity or scale effects). In case exact ranges of values cannot be determined, upper bounding cases might be studied to demonstrate robustness of the repository concept.

All criteria are based on current understanding of the repository system and host rock behaviour, i.e. on a set of gas-related processes, which are often derived from laboratory scale experiments. If progress is made in understanding system performance, the criteria should be adjusted. The current definition of safety function indicators goes back to the first stage of the Sectoral Plan (NTB 08-05) and has since that time not been revised with respect to repository-induced effects, including gas production and transport.

7.1 Porewater Displacement

Two gas-related indicators have been defined by Nagra (NTB 14-14). The first indicator is related to gas pressure induced displacement of porewater (polluted with radionuclides) under visco-capillary two-phase flow conditions. According to Nagra this displacement becomes critical if the induced Darcy flow rate in the host rock exceeds 10^{-11} m/s. Substantial pore water displacements only occur when gas pressures are above the gas entry pressure (capillary threshold pressure). There is a strong sensitivity of gas pressure build-up and water flow from the repository to the intrinsic permeability of the Engineered Gas Transport System EGTS (NTB 16-03, NAB 16-07, NAB 16-08).

7.2 Pathway Dilation

The second indicator used by Nagra is to evaluate the potential for pathway dilation[3]. According to NTB 04-06, pathway dilation occurs when gas pressure is "slightly below the minimal principal stress", and according to NTB 08-05, NTB 08-07 and NTB 14-14, pathway dilation occurs "when the gas pressure reaches 80% of lithostatic pressure". Pathway dilation as investigated by Marschall et al. (2013) occurred at Mont Terri at 2-3 MPa below hydrofrac shut-in pressure (minimum principal stress level), and in the Benken borehole (in a fault) at 3-4 MPa below the minimum principal stress (Nagra 2002).

The 80% magnitude of vertical (or minimal stress) for pathway dilation is not well constrained, considering available lab experiments and in-situ experiments in Opalinus Clay (Chapters 4.2 and 6.2). Considering the tectonic setting of the three potential siting regions and the existing stress measurements in Northern Switzerland (ENSI 33/460) the minimal principal stress is assumed to be subhorizontal and smaller or equal to the overburden stress at repository depth

[3] Pathway dilation is defined by Nagra as gas flow along micro-fractures under dilatant stress and strain conditions (NTB 08-07). According to NEA (1996) pathway dilation has many similarities with the processes of microcrack initiation and propagation.

(Sh/Sv =0.6 to 0.95). In addition, based on lab test results, dilatancy of Opalinus Clay is a function of confining stress and differential stress levels (Chapter 4.1). It is therefore recommended to use other stress components than vertical stress as indicators for pathway dilation and to carefully re-evaluate the threshold values for repository near and far field stress conditions.

7.3 Gas Fracking

Following NTB 04-06, rapid pore pressure build-up, reaching magnitudes of minimal principal stress plus tensile strength, could lead to the formation of new gas-fracs. Short-term tensile strength of saturated Opalinus Clay is low (0.5-1.0 MPa Wild et al. 2015) and might become negligible at long time scales and slow loading rates. Therefore, EGT recommends that tensile strength should not be considered for gas fracking scenarios.

According to Nagra, such scenarios are not expected to occur in an I/LLW repository, where gas pressures caused by the high initial gas production rates (up to 300 m^3 per year and meter of cavern) will be damped by the high initial gas storage capacity and the Engineered Gas Transport System (EGTS) (NTB 16-03, NTB 08-07). Simulated pressures in the base case reach maximum pressures of about 7 MPa (1.5 MPa above hydrostatic) at different locations in a I/LLW repository at 550 m depth. At late times, the gas produced in an I/LLW repository is expected to be released without overpressure formation through the host rock and Engineered Gas Transport System (EGTS). EGT has raised significant concerns related to the long term performance of the EGTS in their evaluation report for SGT Stage 2.

Gas production rates in the HLW repository are assumed to remain at low levels (up to 0.1 m^3 per year and meter of drift) for many thousands of years (Chapter 5.1, NTB 16-03). Following NTB 16-03 highest pressures of about 10 MPa in the HLW emplacement rooms at 700 m depth are expected to occur shortly after emplacement (due to thermal expansion from waste heat production) and after about 10'000 years (due to corrosion gas accumulation in the sealed repository). Based on numerical modelling results for HLW drifts, peak pressures always remain below 80% of lithostatic stress, and are mainly dependent on repository gas/heat generation rates and repository seal (EGTS) permeability (NTB 16-03).

7.4 Gas Leakage and Shearing of Critically Stressed Faults

NTB 04-06 reports the possible migration of gaseous $^{14}CH_4$ and the gas pressure induced advective mobilization of dissolved radionuclides in HLW and L/ILW and concludes that the estimated radiation exposure of the population via such pathways lie below regulatory guidelines by orders of magnitude. NTB 08-07 and NTB 16-03 come to a similar conclusion. However, gas mediated release of gaseous and dissolved radionuclides through reactivated steeply dipping fault zones is not discussed in Nagra reports.

As described in Chapters 2-4, significant gas or brine transport pathways can form along critically stressed fractures and steeply dipping faults in Northern Switzerland, including the potential siting regions. Nagra does not consider gas flow (mainly H_2) along persistent fractures or faults as safety relevant, because it has no direct impact on contaminated pore water displacement (NTB 08-07), and because fractures and faults are supposed to seal efficiently after their formation or reactivation (Marschall et al. 2004). However, sealing of faults in Opalinus Clay has only been empirically assessed, and the new research results from Mont Terri related to the sealing mechanism at field and lab scale and time scales involved are not conclusive (Orellana Espinoza 2018, PhD M. Williams in preperation). Permeability measurements from faults in Mont Terri are controversial and “scaly” fault zones recently investigated in the Belchen Tunnel have significantly elevated permeabilities (Renz et al. 2019).

Reactivation of critically stressed faults requires substantially smaller gas overpressures than pathway dilation and gas fracking, and faults weakened by gas pressure reactivation could be subsequently used for migration of contaminated groundwater. The conditions under which elevated gas pressures can induce fault slip under two-phase conditions have not been studied in detail, but several field cases demonstrate that gas pressure can strongly leak through caprocks of considerable thickness along faults (Chapter 2). As shown by recent fault slip experiments (Guglielmi et al. 2015; Jeanne et al. 2018), activated Opalinus Clay fault rocks have very low shear strength and negligible cohesion under full saturation. In addition, it was shown that small slip events can induce very large changes in fracture transmissivity over fault patches with significant size (Guglielmi et al. 2017). Fault rocks and residual strength of (initially intact) Opalinus Clay samples are characterized by a complete loss of cohesion and low friction angles at stress levels above 3 MPa (Amann et al. 2010, Haug 2009).

It is therefore recommended to investigate (i) conditions for gas leakage along steeply dipping faults, (ii) the conditions for fault zone reactivation under elevated gas pressures, and (iii) the impacts of gas-pressure mediated radionuclide migration through reactivated fault zones on long term safety. We recommend to consider the fault reactivation potential as an additional safety indicator.

8. Summary of Recommendations

8.1 Preamble

EGT considers steeply and predominantly NNE-SSW striking strike-slip faults as relevant for gas-pressure buildup, gas transport and possibly also radionuclide migration from the HLW and I/LLW repositories. These faults also play a major role for the repository placement within a siting region, the detailed repository drift layout, the emplacement of wastes within a given drift or cavern, the barrier concept, and the design and location of individual sealing systems. EGT considers the current knowledge of in-situ properties of such faults, occurring at multiple scales within all proposed siting regions and the effective containment rock zones, as very limited and insufficient. Representative in-situ properties including structure, stress, pore pressure, 2-phase flow conditions and hydro-mechanical coupled strength of Opalinus Clay can only be derived through inclined core drillings. The currently planned boreholes at the proposed siting regions are all vertical and will only rarely intersect steeply dipping faults.

Due to the large spatial variability of fault densities and structural properties at all scales, reliable site-specific differences in safety-relevant fault properties might not be acquired from a few inclined drillings at the proposed sites, i.e. for site selection. On the other hand, EGT considers very important the characterization of critical properties of such faults within the Opalinus Clay at the selected site for safety assessment and repository layout (including EGTS). As such fault properties and their uncertainties need to be critically considered both for the quantitative and qualitative assessment of long term safety. Considering the poor knowledge of information on these strike-slip (and transtensional) faults within the Opalinus Clay at depth, a program for a quantitative understanding of fault properties and related gas and brine transport processes is considered important. As these properties are considered safety and layout relevant, their properties should be determined in a robust way for the general license application. Robust implies for EGT, that a representative number of faults at multiple scales should be investigated at representative locations. EGT expects, that this goal can not be achieved with the currently planned vertical boreholes only.

8.2 Detailed recommendations of EGT

1. Characterization of the spacing, fabric and hydro-mechanical properties of steeply dipping faults within the Opalinus Clay at the depth of the repository requires additional investigations and observations that include (1) reprocessing and evaluation of seismic attributes, (2) additional 3D-VSP measurements in each siting region and (3) intersection and testing of these faults with vertical and deviated boreholes. If these data are not or only partially available for site selection, the deficiency of data should be reflected in a comprehensive assessment of uncertainties in SGT criteria 3.2 and 3.3. For the general license application EGT recommends to carry out a representative number of in-situ investigations of steeply dipping faults at multiple scales with vertical and inclined boreholes.
2. Only very few experiments have investigated fault strength properties of Opalinus Clay, especially considering the stress and consolidation history in the repository siting regions. In addition, Opalinus Clay shows a strong dependence of its strength and stiffness properties on saturation, and it is expected that fault reactivation in Opalinus Clay by gas pressure build-up cannot be adequately assessed from fully saturated experimental conditions. This also holds for fault zones, where pore sizes and fracture aper-

tures require capillary forces to be considered. It is therefore recommended to investigate fault rock strength properties and conditions for fault reactivation under fully saturated and partially saturated conditions with specific lab and field experiments.

3. Loading of the repository near-field by gas pressure is a long-term process, and a better understanding of the long-term strength and deformability of the brittle-ductile Opalinus Clay is potentially also a key behavioural aspect for long-term safety that should be studied further.
4. Thermal impact on processes in the L/ILW is not considered by Nagra (NTB 16-03, p. 25). In case of co-disposal concepts, the thermal field of the HLW repository may induce a temperature increase in the L/ILW facility. Respective consequences on gas evolution scenarios should be discussed. While the abiotic anaerobic corrosion of iron is found to be less temperature dependent (e.g. Féron und Crusset 2014), this is different for degradation of organic components and microbially induced processes. Potential consequences of thermal effects on gas evolution in L/ILW evolution scenarios for co-disposal concepts should be discussed.
5. The two-phase flow properties and processes of Opalinus Clay under realistic heterogeneous conditions are poorly understood. Therefore we recommend four important fields of further analysis: (i) Finding further experimental evidence on the connectivity of pores and microcracks under changing mechanical, hydraulic, and thermal conditions to identify major factors of influence for a suitable parameterization to be used in predictive numerical simulation models, (ii) improving the understanding of flow regimes from Lenormand und Zarcone (1989), (iii) investigating the two-phase flow conditions of macro-fractures and fault zone, and (iv) testing the application of percolation models to proceed towards a more realistic description of capillary fingering regimes. This will require including stochastic approaches to complement deterministic simulations in an appropriate way, aiming at quantifying the uncertainties arising from unknown details and variability of sub-REV-scale pore connectivity.
6. The 80% magnitude of vertical (or minimal stress) for pathway dilation is not well constrained, considering available laboratory and in-situ experiments in Opalinus Clay. Considering the tectonic setting of the three potential siting regions and the existing stress measurements in Northern Switzerland (ENSI 33/460), the minimal principal stress is assumed to be subhorizontal and smaller or equal to the overburden stress at repository depth (Sh/Sv = 0.6 to 0.95). In addition, based on laboratory test results, dilatancy of Opalinus Clay is a function of confining stress and differential stress levels. It is therefore recommended to use other stress components than vertical stress as indicators for pathway dilation and to carefully re-evaluate the threshold values for repository near and far field stress conditions.
7. As described in Sections 2-4, significant gas or brine transport pathways can form along critically stressed fractures and steeply dipping faults in Northern Switzerland, including the potential siting regions. Reactivation of critically stressed faults requires smaller gas overpressures than pathway dilation and gas fracking, and faults weakened by gas pressure reactivation could be subsequently used for migration of contaminated groundwater. It is therefore recommended to investigate (i) conditions for gas leakage along steeply dipping faults, (ii) the conditions for fault zone reactivation under elevated gas pressures, and (iii) the impacts of gas-pressure mediated radionuclide migration through reactivated fault zones on long term safety. We recommend considering the fault reactivation potential as an additional safety indicator.

All items in this report refer to the HLW as well as the I/LLW repository. N-S- to NNE-SSW-oriented strike slip faults should be considered critical for gas and brine transport, and therefore for site evaluations, repository layout (with Engineered Gas Transport Systems) and repository performance assessment.

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Appendix

Critical Evaluation of Gas Transport Mechanisms, Scale Dependencies and Gas-Rock Interactions in the Opalinus Clay (Dr. Russell Johns)

CRITICAL EVALUATION OF NAGRA REPORTS ON GAS TRANSPORT MECHANISMS, SCALE DEPENDENCIES, AND GAS-ROCK INTERACTIONS IN THE OPALINUS CLAY

SUBMITTED TO SWISS FEDERAL NUCLEAR SAFETY INSPECTORATE ENSI, OCTOBER 25TH 2019

BY DR. RUSSELL JOHNS

Executive Summary

This report provides a critical evaluation of the Nagra technical reports on gas transport mechanisms, scale dependencies, and gas-rock interactions for the Opalinus clay as a potential spent fuel, intermediate and high-level nuclear waste repository (SF/ILW/HLW). Specifically, this evaluation is based on Chapter 3 in three NTB reports 04-06, 08-07, and the NAB report 13-83. Critical comments related to these documents are given in approximate order of their discussion in the reports.

Overall, classical concepts of multiphase flow and diffusion are described well in the reports, but it is likely that geomechanics, nonisothermal multiphase flow with adsorption, surface reactions, and potentially other transport mechanisms should be coupled together in complex simulations that mimic the planned activity at the end of the operational phase and after closure. More physical relative permeability and capillary pressure models should be used than are used in the simulations presented in these reports.

This evaluation recognizes that it is relatively easy to be critical of other's work, so the goal here is to be as constructive as possible, while making it clear when there could be improvements.

Introduction

The Opalinus clay (OPA) is the likely repository for nuclear waste in Switzerland. After emplacement, hydrogen gas and heat will be generated over time, creating the potential for pressure buildup and transport of radioactive material to the surface. Gas transport mechanisms could include advection, diffusion, surface processes, adsorption, retardation, dissolution in brine, and other driving forces. Properties from the lab must be scaled up to the field to account for heterogeneities, time-dependent and equilibrium surface reactions, fractures initially present, microfractures that form as pressure is gradually increased (dilatancy), and macro-scale fractures that may form when fracture pressure is exceeded. Further, gas-rock interactions will be very important to transport, which can include relative permeability and capillary pressure functions.

Classically, there are three groups of properties that are important in porous media flows and transport. The key fluid properties are density, pressure, temperature, viscosity, compressibility, heat capacity, and composition. The key rock properties are heat capacity, overburden (rock density), strength/stress, permeability, and effective porosity. There are also rock-fluid interactions, such as capillary pressure, relative permeability, chemical reactions at the rock surface and within a phase, and adsorption/desorption. Many of these properties are averaged properties, such as permeability and capillary pressure. Macroscopic properties likely do not apply for rock pores < 5 nm and instead these properties must be modelled statistically. However, as stated in the NAGRA reports, it is likely that the larger pores are the main contributor to gas transport so use of macroscopic averaged properties is appropriate.

Hydrogen gas is generated following emplacement in the engineered barrier system (EBS). The ultimate gas release from the EBS to the surface owing to SF/ILW/HLW depends on transport through the backfill and tunnel seals, cementitious materials, and the geosphere. Microscale fractures that form during the process and macroscale fractures that may already be present (or might form when fracture pressure is exceeded) will likely form the fast path for gas, and hence radioactive isotopes to escape through the geosphere to the biosphere. The potential for dilatant microcracks to form is likely dependent on the rate of gas generation and whether pressure buildups fast or slow, which depends on gas generation and the ability of gas to leak off from the repository zone. Transport of gas with time is therefore one of the critical aspects to consider, which depends on the fluid, rock, and rock-fluid interaction properties of the engineered and natural barriers (canisters, backfill, and cement material).

Common transport mechanisms for the generated gas are advection and diffusion of gas dissolved in brine. Hydrogen has a very small solubility in brine, but for the time scales considered here this could be an important way for transport of dissolved gas by advection and diffusion. If the gas builds up significantly to form a vapor phase, the vapor phase can move by advection through the porous media once the entry pressure is exceeded. This assumes generated gas buildups sufficient pressure so that it displaces the wetting phase, which is assumed here to be water. Critical gas saturation is only relevant if gas evolves from the brine as pressure is lowered, but this saturation is likely small. Gravity through buoyancy can also serve to increase the rate of transport of the gas to the surface. Gas transport to the biosphere can be delayed by adsorption within a porous media. Adsorption effects are likely significant in the geosphere with large specific surface area (SSA, surface area divided by volume). Surface reactions are also much more important in ultra-tight (low permeability) rocks with large SSA and there is a potential for bioreactions (bacterial growth) that can produce hydrogen sulfide and degrade cement, while plugging the pore throats at the repository boundaries and in the backfill.

Besides these classical transport mechanisms, transport within a porous media can have many more mechanisms as shown in **Figure 1**. This may be especially true in ultra-tight rocks where the fluids can interact at the nanometer (nm) scale with the surfaces of the rock. For example, the impact of stress is more important in low permeability porous media than in high permeability. That is, the relatively change in permeability/porosity with increasing (or decreasing) effective stress is much greater in low permeability rock. Fractures can open and close significantly based on stress changes. Further, clays can act as a membrane causing osmotic pressure differences. Significant research is needed to understand these coupled interactions as depicted in Figure 1. Most petroleum and groundwater engineers typically resort to the classical mechanisms because most software is available to model only these mechanisms. Figure 1 is not intended to imply that all mechanisms must be considered in detail, but perhaps relevant mechanisms should be reviewed qualitatively.

The petroleum industry is starting to recognize that surface diffusion may be an important mechanism for recovery especially where solvent (say methane) is injected in a "huff" period, followed by a "puff" period where production occurs in the same well. Although diffusion is a slow process, a complex network of hydraulic fractures are generated during "fracking" in shale reservoirs making a large contact area between the fracture surfaces and tight matrix rock. Thus, the diffusion process can be enhanced through the significant contact area. Fractures are likely always dominated by advective transport, but the impact of stress on their creation, growth, and evolution is critical.

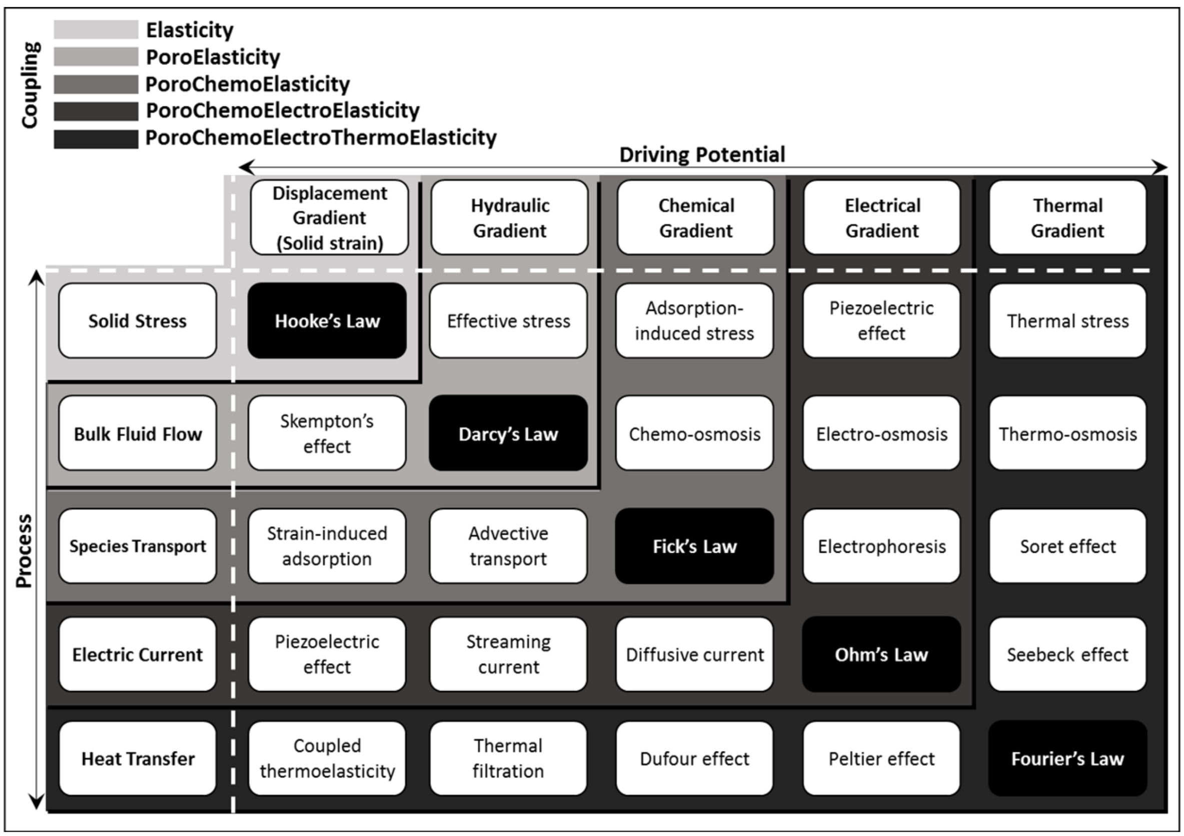

Figure 1 Illustration of potential transport mechanisms in porous media and in engineering in general. Modified by A. Mehrabian and R. Johns (2018). Mechanisms such as Ohm's law and Fourier's law do not need to be considered for porous media.

Critical Evaluation of NTB Reports 04-06, 08-07, and NAB report 13-83

The Nagra reports have significant repetition in them. Thus, comments here relate mostly to the first report, NTB 04-06. Comments are then made for new points that are only in the last two reports. For expediency, references are only given in this report when they are not mentioned in the Nagra reports.

1. Table 3.1-1 gives a very limited set of possible transport mechanisms of released gas and concludes that both advective and diffusive transport is likely small in tight rocks. While these are likely the dominant mechanisms, it would be useful to evaluate other transport mechanisms shown in Figure 1 above.
2. Diffusive transport could be enhanced from what is described here owing to formation of microcracks that could increase the contact area between the dissolved gas and water in the tight rock. Diffusion cannot be correctly modelled in numerical codes unless the grid-block sizes are very small and the contact area is correctly modelled with time (contact area increases with time as cracks grow). The inclusion of increased permeability owing to dilatancy-controlled leakage will likely underestimate the impact of diffusion because the contact area between the microcracks and the tight rock is not explicitly accounted for in the simulations.
3. The impact of increased temperature on transport is only briefly mentioned in the report, but this could be significant for transport. High temperature coupled with gas transport could also impact the fractures especially if the rock becomes dry (either at the time of the operational phase or after closure). Rock near the emplacement could become more brittle decreasing the tensile strength of the rock and thereby increasing the risk of fracturing. The reports did not specifically discuss change in rock strength with saturation. Rock strength tests should be performed according to the expected anisotropic stresses and saturation conditions.
4. Numerical simulations should be done that couple geomechanics to nonisothermal flow and transport. Although very complex to perform, these simulations could be done at various scales to identify the most important mechanisms and the structure/impact of microcracks and macrofractures on transport. The report presents empirical relationships only for permeability increase with time. Such empirical relationships are typical in porous media, but for the time scales involved here detailed geomechanical simulations coupled to flow and transport should be done.
5. Diffusion is related to chemical potentials as shown in Bird, Stewart, and Lightfoot (2007). Diffusion of hydrogen within the brine phase appears to be treated using a simple Fickian form, although diffusion is more complicated. Firoozabadi (2015) [p. 334] shows that multicomponent diffusion flux can be expressed in terms of a combination of Fickian (molecular) diffusion coefficients ($\boldsymbol{D}^M$), thermal diffusion coefficients ($\boldsymbol{D}^T$), and pressure diffusion ($\boldsymbol{D}^P$) in a compact manner as:

$$\vec{J}_{Di} = -c(\boldsymbol{D}^M \cdot \nabla x + \boldsymbol{D}^T \nabla T + \boldsymbol{D}^P \nabla P),$$

   where diffusion coefficients reflect non-ideal fluid properties and interactions between components. The three terms in the above eqaution are molecular diffusion, pressure diffusion, and thermal diffusion, respectively [Firoozabadi (2015), p. 336]. The above expression for flux, however, is written only for diffusive flux of a bulk fluid. This flux is then corrected for a porous medium by decreasing the effective area over which mass flux can occur and then by increasing the average length travelled a particle must move around rock surfaces by introducing tortuosity. It is not clear, however, what happens to these equations when the size of pores approach the nanometer scale. At tens or hundreds of nm's, the mean path length of a random molecular jump exceeds the dimensions of the porous media so that interactions with the rock surface become important. This is sometimes called Knudson diffusion, although this type of diffusion will likely not occur for dense fluids at high pressure.

Fractures if present/created would be the main pathway for gas movement. Microcracks may increase diffusion through increased contact surface area. Diffusion could reduce the pressure of the gas as hydrogen diffuses away.

6. The reports do not discuss the impact of gravity as a driving force owing to buoyance of the gaseous phase. Hydrogen gas will likely move upward through fractures.
7. Capillary pressure will be very large between the gaseous and aqueous phase within the tight rock matrix (gas pressure will exceed water pressure), while capillary pressures in fractures will be small (water pressure equals gas pressure). It is not clear which pressure (gas or water) is important to determining whether fractures are created. If gas is in the center of the pores (water is completely wetting the surface as indicated by a contact angle of zero), then the pressure of interest for stress calculations would likely be the water pressure that must exceed the fracture pressure. If the contact angle changes so that gas contacts some of the rock surface, then the gas pressure might be important. The report appears to assume that gas pressure is the pressure that determines fracture generation. Contact angles should be measured for a hydrogen/brine/rock system where the rock lithology could be varied, although the rock is likely highly water wet.
8. The report does not mention viscosity of the fluid, but mobility (effective permeability divided by viscosity) governs two-phase advective transport. A high mobility fluid (gas) will flow faster than a low mobility fluid (water) at the same saturation. The report mentions that gas mobility is primarily controlled by the intrinsic permeability. This phrasing is not accurate. Mobility of any phase can be written as the effective permeability divided by viscosity of that fluid, where effective permeability is the intrinsic (or absolute) permeability multiplied by the relative permeability (mobility of phase *j* = kk_{rj} / μ_j). The intrinsic permeability will impact both the gas and aqueous phases, not just the gas mobility. The fraction of the total flow that is gas, for example, is from Darcy's law for two-phase flow of gas and water $f_g = kk_{rg} / \mu_g \Big/ \left(kk_{rg} / \mu_g + kk_{rw} / \mu_w \right) = \lambda_g \Big/ \left(\lambda_g + \lambda_w \right)$. The relative mobility λ_j of phase *j* is thus most critical for determining the flow rate of a phase, where $\lambda_j = k_{rj} \big/ \mu_j$. The intrinsic permeability cancels out of the fractional flow equation above.
9. The Van Genuchten (VG) model for capillary pressure accurately represents capillary pressure in soils, but should never be used for consolidated rock and especially for tight rock. The report describes that gas will enter at low pressure owing to the VG model, but this is not physical as there should be a finite entry pressure based on the largest pore throat size in consolidated rocks. This is a common misconception observed in much of the groundwater literature. This misconception likely emanates from the difficulty of measuring capillary pressure curves on unconsolidated porous media. Brooks-Corey (BC) capillary pressure model should be used because it gives a realistic finite entry pressure when matched to data. This could potentially change the "leak off" of gas into the rock as this entry pressure must be exceeded before gas would enter a water saturated rock. The NAB report 13-83 did mention use of the BC model for some of the boundary formations. Further, Figure 3-29 shows correct capillary pressure-corrected measurements from the petroleum industry and therefore finite entry pressures.

   The discrepancy is likely related to not making the needed corrections of the experimental data. Capillary pressure curves measured in a lab must be corrected by the closure volume. Plugs cut from cores have irregular surfaces that allow for an apparent low entry pressure of the injected fluid. This entry pressure is not real. In some cases, part of the core plug may have grains that fall off that give a very large "pore" on the surface. In such cases, that portion of the core can be sealed off using epoxy. Even after these effects are accounted for, one must correct for the volume needed to "enclose" the core plug sample. That is, a "closure" correction must be made to the cell-corrected volume injected to account for roughness around the core sample that is not related to the pore structure of the rock. The estimated closure volume must be subtracted from the cell-corrected volume data. Given sufficient data, the volume at which closure occurs can be estimated at the inflection point from a plot of the injection pressure as a function of the difference between the volume injected and the empty cell volume. The cell volume is also typically corrected for various pressures. Once properly corrected, there will be a finite entry pressure for consolidated samples and for gas-water in tight rocks this pressure will be large.

The VG curve allows some gas to leak off at pressures below the entry pressure. Simulations should only be made with realistic entry pressures. The sentence in the report "Hence, the porous media is not characterized by a sharp capillary threshold value" is simply an outcome of the VG model and is not correct for consolidated tight rocks.

10. There is significant confusion in the reports on what the critical gas saturation is compared to residual gas saturation. Normally, the critical gas saturation is used in the oil industry to represent gas that evolves from the oil, i.e. when the pressure drops below the bubble-point pressure of the oil. This gas buildups in the center of the pores (if gas is nonwetting) and will not flow until a critical gas saturation is reached. This is not likely to occur in the rocks described here, as the water contains little gas (solubility is low), and the pressure must be reduced so that the water can no longer hold the gas. Typical values of critical gas saturation can vary from as low as 0.05 to around 0.30 in tighter rocks within the petroleum industry. Figure 2 taken from the oil industry for gas-oil systems demonstrates the difference between critical gas saturation and trapped gas (or residual gas) saturation. In this figure, oil and connate water saturation can be lumped into one wetting phase. Figure 3-6 in NTB 08-07 appears to have similar curves to this, showing a finite relative permeability at water saturations near 1.0. However, the value of S_{gr} in that figure is not clear.

    Residual gas saturation is not related to critical gas saturation, although the reports imply this is the case. To understand this concept, consider draining the water (assumed the wetting phase here) from a porous media by injecting gas into the rock until a maximum gas saturation is reached as determined by the maximum gas injection pressure applied. Then, water is imbibed into the rock (or is injected in). When water is completely wetting it will follow the same path along the surfaces of the rock and therefore show no hysteresis. Snap off of the gas phase occurs in the pore throats where water moves around the gas. Gas in the larger pores can also be bypassed by smaller pore passages. Both of these cause a certain amount of trapped gas during the imbibition process – this is known as the trapped gas saturation, or in this report the residual gas saturation. Thus, one must have hysteresis (gas injection followed by water imbibition) to obtain a residual gas saturation. The statement regarding the experimental observation that the critical gas saturation is higher than the residual gas saturation from the Dury et al. (1999) paper confuses the issue further and is likely unphysical for a variety of reasons.

    The report implies that critical gas saturation and residual gas saturation are similar. They are not as described above. For the gas threshold tests, for example, gas will flow into the porous medium when the gas pressure exceeds the entry pressure of the pore throats. Thus, there is no critical gas saturation as gas enters the rock – it will move in if pressure is sufficient to overcome the capillary pressure of the next largest pore throat. Relative permeability therefore must be described properly by using both a drainage and imbibition curve. Gas relative permeability will be nonzero for gas saturations approach zero when the rock undergoes drainage (again assuming gas is completely nonwetting). Scanning curves should also be used if one expects multiple cycles of drainage and imbibition.

11. The Mualem model for relative permeability is derived partly based on the VG model. This model uses a normalized or effective saturation (S_e) where the residual gas saturation is used. Thus, this is an imbibition model only and should not be used for drainage if that is to be modelled. The water saturation in this case cannot become greater than $1 - S_{gr}$ as the effective saturation varies from 0 to 1.0.
12. The Nagra reports use the phrase "gas imbibition tests". This phrase is confusing as only water imbibes if water is the wetting phase. I assume here that water will generally be the wetting phase in the OPA, but again the contact angle should be measured using the actual brine and hydrogen gas on the clay surface. If the water is not completely wetting, the relative permeability curves for both drainage and imbibition should be measured (or estimated from PSD's) along with the trapped gas saturation.
13. Relative permeability and capillary pressure curves will change with the structure of the pores in the porous medium. Because the OPA is very tight it would be reasonable to assume the OPA is fairly homogeneous because fractures within the OPA will provide the fast path for flow. At the boundaries between the OPA and the repository, however, the porous media structure will change (bentonite to OPA for example, or by the EDZ – disturbed zone) causing a discontinuous saturation jump owing to capillary pressure continuity there. It is not clear this effect was modelled in the simulations, which could be important, as is described in an internal Nagra report by Georg Resele and myself around 1994. That report gives an analytical solution for vertical gas movement in an old borehole, but the principle is the same. This effect is also well known in the oil industry and is typically called the capillary end effect caused by exposure of a core plug end to atmospheric pressure (air). To simulate this effect here, the boundary area must be refined with very small grid blocks. Upscaling of this effect is very difficult to do accurately.
14. Adsorption of hydrogen and water appears to not be included in the simulations, although I do see mention of water adsorption on the capillary pressure function. I would expect adsorption to be significant in the OPA owing to its high specific surface area.
15. As stated in the report, fractures likely heal as pressure is reduced. It may be possible though that some shear exists in generated fractures close to the repository so that fractures cannot close perfectly. This should be examined in a coupled geomechanical/fluid model.
16. Microcracks will be difficult to model without using an enhanced permeability value, as is done in the Nagra reports. The increased contact area for diffusion caused by the microcracks is best modeled using the concept of dispersion, which is widely used in the groundwater literature. How much "dispersion" to use to enhance diffusion depends largely on the intensity of the microcracks. Numerical dispersion can overwhelm diffusion if grid blocks are too large. Thus, it is recommended to match the expected physical dispersion (enhanced diffusion level) by the appropriate grid-block size. The alternative is to use very small grid blocks with input dispersivity.

17. The statements “hydro-frac methods used in hydrocarbon exploration to permanently increase the permeability” is somewhat misleading. Hydraulic fracturing opens natural fractures present and creates new macrofractures. There may also be numerous microfractures that “shatter” the shale, although that term is only descriptive. The goal here is to increase the contact area as much as possible between the high permeability fractures and the ultra-tight shale matrix so that oil can be effectively produced. Gas is also injected into the fractures in a huff’n’puff scheme (alternating injection/production periods) whereby it likely diffuses into the tight matrix causing counter diffusion of oil.
18. NTB 08-07 discusses up-scaling of single-phase diffusion and multiphase flow. Upscaling of diffusion was discussed in point 16 above. Scaling up multiphase flow is much more complex than for diffusion. Subramanian et al. (1999) developed 1-D analytical solutions of series flow through two heterogeneous layers for binary displacements. That work showed that it is not possible to scale up multiphase flow owing to fractional flow continuity that creates a dynamic saturation jump at the boundary between two porous media (that have different relative permeability functions). Dynamic changes in properties would have to be used, which is not practical in numerical simulation. Although it is not accurate, there is no choice but to upscale relative permeability when large grid blocks are required, but the best choice is to use the most refined grid possible.
19. There is no agreement in the petroleum industry that Darcy’s law is not valid for large pressure gradients in low-permeability porous media, as is indicated in NTB 08-07 in Section 3.2.1. Instead it could be that other forms of transport are the cause for the discrepancy in the experiments.
20. Khorsandi et al. 2017 and Purswani et al. 2018 have developed a new type of petrophysical model for relative permeability and capillary pressure in porous media. This approach is based on mathematical state functions that allow for relative permeability (and capillary pressure based on similar inputs) to vary continuously and uniquely based on inputs such as saturation, wetting angle, Euler characteristic (that describes the connectivity within a phase), capillary number (likely not important for the OPA unless interfacial tension changes significantly), and pore structure characteristics. The advantage of this approach is that these rock-fluid interactions are physical and can be tuned to experimental data so that these properties can be predicted away from the measured data. Further, hysteresis is easy to model in this approach, which is not true of current empirical methods. The disadvantage is that the approach is new and more benchmarking is needed and the approach has yet to be implemented in a commercial simulator. The methodology may prove useful, however, to understand better how these rock-fluid interactions vary and also how residual saturations can change within a porous medium, i.e. there is not one value of residual gas saturation in a porous media for example, but its value depends on the endpoints of the paths taken (hysteresis).
21. NTB 08-07 discusses the drying of the rock zone around the underground structure during the operational phase of the repository. It is likely that after closure gas will be trapped by an imbibition process (assuming water wet clay) for some time owing to low solubility of air (and hydrogen) in water. It is not clear, however, how long it will take (by diffusion and by any groundwater flow across the zone no matter how small) before air is solubilized completely before hydrogen is generated. Assuming hydrogen is generated while gas is trapped, then the initial process is an imbibition one, followed by drainage of water as hydrogen is generated. Once no more hydrogen is generated, water could come back in a second imbibition cycle. The process could be quite complex depending on the timing of these events and only simulation with coupled physical transport mechanisms (potentially some of those shown in Figure 1) and use of a physical relative permeability/capillary pressure model

could provide sensitivities to that timing. The function f_g in Eq. 3-10 of NTB 08-07 as well as the term "dynamic relative permeability" is likely the result of an improper physical model and/or relative permeability heterogeneity.

22. Spreading of the saturation distribution is not a mixing effect as described in the NTB reports and cannot be described by a dispersive flux term, as discussed in point 18 above. Saturation spreading is the result of capillary pressure and also results from different velocities of a fixed saturation based on classical Buckley-Leverett (BL) displacement theory in the petroleum industry.
23. Surface reactions add additional significant complexity and uncertainty to the simulations of the transport of gas away from the repository. These are discussed well in Section 3.4.2, although there is no mention of the potential for bacterial growth blocking flow and transport in the Nagra reports. Sulphate reducing bacteria produce hydrogen sulfide, which can degrade concrete, but if their populations grow before they cease this could potentially seal the cement zone and/or neighboring rock causing greater pressure buildup during hydrogen generation. The repository environment is likely not conducive to growth hundreds of years post closure, but there might be the opportunity for growth prior. This is outside of my direct research area, but bacterial growth causing hydrogen sulfide is a substantial problem in the oil business that can corrode well casings and pipes.

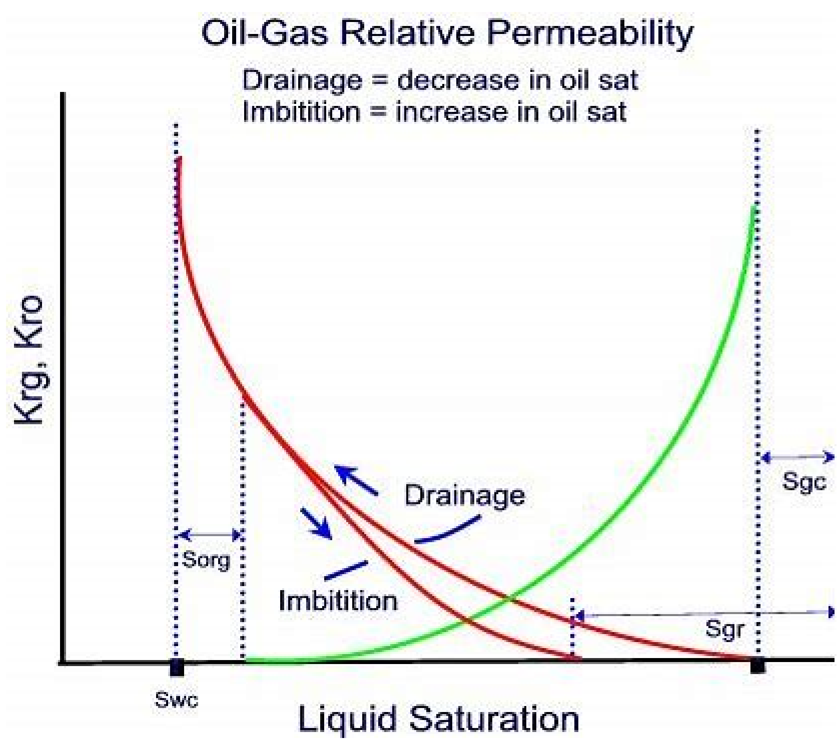

Figure 2: Illustration of the difference between residual gas saturation (trapped saturation) and critical gas saturation (from petrocenter.com). Oil and connate water is the wetting phase here, while gas is the nonwetting phase. Water is present at the connate water saturation, but it is not flowing (water and oil can be lumped together as the wetting phase shown as liquid saturation). Critical gas saturation applies only to the gas relative permeability curve under drainage of the wetting phase (as gas evolves from oil), while residual gas saturation (or trapped gas) applies only for imbibition of the wetting phase.

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